

06/25/2006 10824731.trn

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSSPTA1626GMS

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * Welcome to STN International * * * * *

NEWS	1		Web Page URLs for STN Seminar Schedule - N. America
NEWS	2		"Ask CAS" for self-help around the clock
NEWS	3	JAN 17	Pre-1988 INPI data added to MARPAT
NEWS	4	FEB 21	STN AnaVist, Version 1.1, lets you share your STN AnaVist visualization results
NEWS	5	FEB 22	The IPC thesaurus added to additional patent databases on STN
NEWS	6	FEB 22	Updates in EPFULL; IPC 8 enhancements added
NEWS	7	FEB 27	New STN AnaVist pricing effective March 1, 2006
NEWS	8	MAR 03	Updates in PATDPA; addition of IPC 8 data without attributes
NEWS	9	MAR 22	EMBASE is now updated on a daily basis
NEWS	10	APR 03	New IPC 8 fields and IPC thesaurus added to PATDPAFULL
NEWS	11	APR 03	Bibliographic data updates resume; new IPC 8 fields and IPC thesaurus added in PCTFULL
NEWS	12	APR 04	STN AnaVist \$500 visualization usage credit offered
NEWS	13	APR 12	LINSPEC, learning database for INSPEC, reloaded and enhanced
NEWS	14	APR 12	Improved structure highlighting in FQHIT and QHIT display in MARPAT
NEWS	15	APR 12	Derwent World Patents Index to be reloaded and enhanced during second quarter; strategies may be affected
NEWS	16	MAY 10	CA/CAPLUS enhanced with 1900-1906 U.S. patent records
NEWS	17	MAY 11	KOREAPAT updates resume
NEWS	18	MAY 19	Derwent World Patents Index to be reloaded and enhanced
NEWS	19	MAY 30	IPC 8 Rolled-up Core codes added to CA/CAPLUS and USPTFULL/USPAT2
NEWS	20	MAY 30	The F-Term thesaurus is now available in CA/CAPLUS
NEWS	21	JUN 02	The first reclassification of IPC codes now complete in INPADOC
NEWS EXPRESS			FEBRUARY 15 CURRENT VERSION FOR WINDOWS IS V8.01a, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 19 DECEMBER 2005. V8.0 AND V8.01 USERS CAN OBTAIN THE UPGRADE TO V8.01a AT http://download.cas.org/express/v8.0-Discover/
NEWS HOURS			STN Operating Hours Plus Help Desk Availability
NEWS LOGIN			Welcome Banner and News Items
NEWS IPC8			For general information regarding STN implementation of IPC 8
NEWS X25			X.25 communication option no longer available after June 2006

Enter NEWS followed by the item number or name to see news on that specific topic.

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* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 11:58:23 ON 25 JUN 2006

=>

Uploading

THIS COMMAND NOT AVAILABLE IN THE CURRENT FILE

Do you want to switch to the Registry File?

Choice (Y/n):

Switching to the Registry File...

Some commands only work in certain files. For example, the EXPAND command can only be used to look at the index in a file which has an index. Enter "HELP COMMANDS" at an arrow prompt (=>) for a list of commands which can be used in this file.

=> FILE REGISTRY

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 11:58:36 ON 25 JUN 2006

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 23 JUN 2006 HIGHEST RN 889213-08-5

DICTIONARY FILE UPDATES: 23 JUN 2006 HIGHEST RN 889213-08-5

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

*
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
*

Structure search iteration limits have been increased. See HELP SLIMITS for details.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information

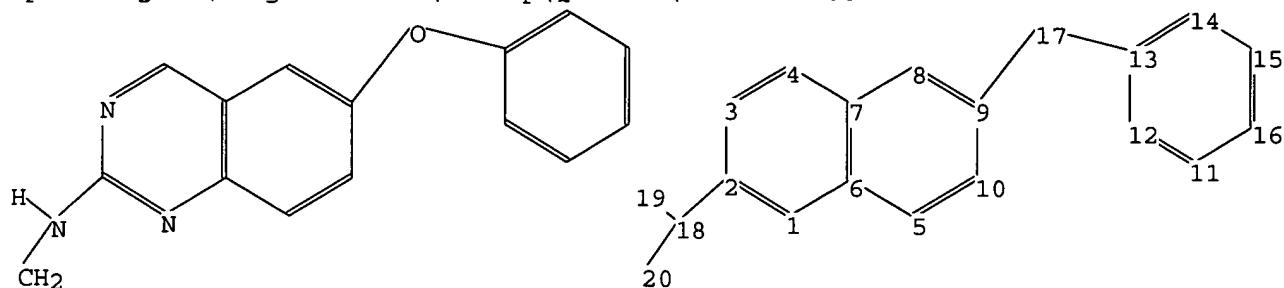
06/25/2006 10824731.trn

on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10824731.str



chain nodes :

17 18 19 20

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16

chain bonds :

2-18 9-17 13-17 18-19 18-20

ring bonds :

1-2 1-6 2-3 3-4 4-7 5-6 5-10 6-7 7-8 8-9 9-10 11-12 11-16 12-13 13-14
14-15 15-16

exact/norm bonds :

2-18 9-17 13-17

exact bonds :

18-19 18-20

normalized bonds :

1-2 1-6 2-3 3-4 4-7 5-6 5-10 6-7 7-8 8-9 9-10 11-12 11-16 12-13 13-14
14-15 15-16

isolated ring systems :

containing 1 : 11 :

Match level :

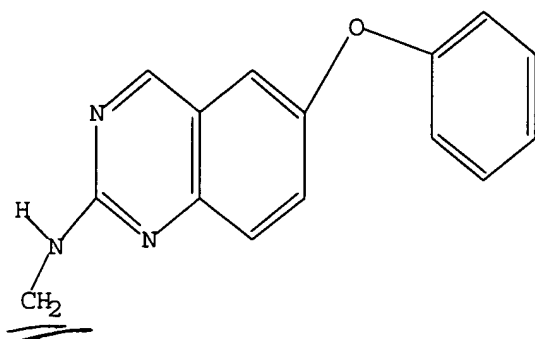
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:CLASS 18:CLASS 19:CLASS
20:CLASS

L1 STRUCTURE UPLOADED

=> d 11

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 11:58:50 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 12 TO ITERATE

100.0% PROCESSED 12 ITERATIONS
SEARCH TIME: 00.00.01

1 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

PROJECTED ITERATIONS: 33 TO 447
PROJECTED ANSWERS: 1 TO 80

L2 1 SEA SSS SAM L1

=> s l1 sss full

FULL SEARCH INITIATED 11:58:56 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 160 TO ITERATE

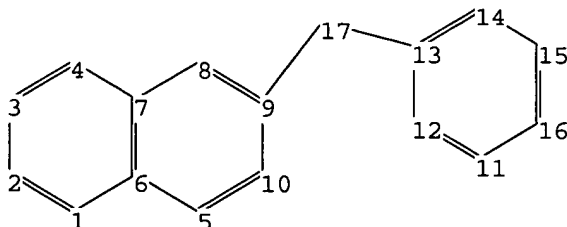
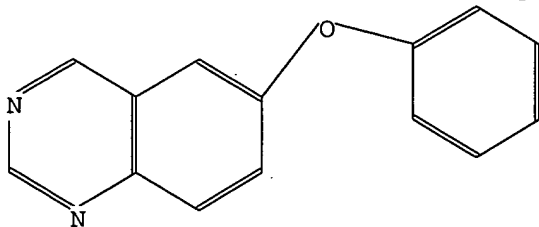
100.0% PROCESSED 160 ITERATIONS
SEARCH TIME: 00.00.01

3 ANSWERS

L3 3 SEA SSS FUL L1

=>

Uploading C:\Program Files\Stnexp\Queries\10824731a.str



chain nodes :

17

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16

chain bonds :

9-17 13-17

06/25/2006 10824731.trn

ring bonds :

1-2 1-6 2-3 3-4 4-7 5-6 5-10 6-7 7-8 8-9 9-10 11-12 11-16 12-13 13-14
14-15 15-16

exact/norm bonds :

9-17 13-17

normalized bonds :

1-2 1-6 2-3 3-4 4-7 5-6 5-10 6-7 7-8 8-9 9-10 11-12 11-16 12-13 13-14
14-15 15-16

isolated ring systems :

containing 1 : 11 :

Match level :

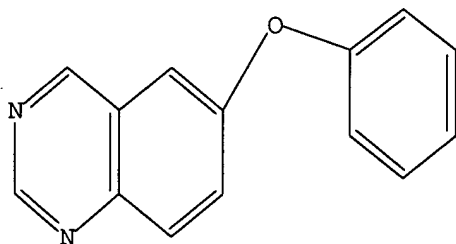
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:CLASS

L4 STRUCTURE UPLOADED

=> d 14

L4 HAS NO ANSWERS

L4 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 14

SAMPLE SEARCH INITIATED 12:00:03 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 260 TO ITERATE

100.0% PROCESSED 260 ITERATIONS

11 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 4233 TO 6167

PROJECTED ANSWERS: 22 TO 418

L5 11 SEA SSS SAM L4

=> s 14 sss full

FULL SEARCH INITIATED 12:00:09 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 5002 TO ITERATE

100.0% PROCESSED 5002 ITERATIONS

SEARCH TIME: 00.00.01

170 ANSWERS

L6 170 SEA SSS FUL L4

=> ~~FIL HCAPLUS~~
~~COST~~ IN U.S. DOLLARS

	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	334.32	334.53

FILE 'HCAPLUS' ENTERED AT 12:00:18 ON 25 JUN 2006
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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FILE COVERS 1907 - 25 Jun 2006 VOL 145 ISS 1
FILE LAST UPDATED: 23 Jun 2006 (20060623/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 13

L7 2 L3

=> s 16

L8 35 L6

=> s 18 and py<=2003

23861848 PY<=2003

L9 28 L8 AND PY<=2003

=> s 19 and p38 kinase

12541 P38

266776 KINASE

52258 KINASES

275331 KINASE

(KINASE OR KINASES)

2825 P38 KINASE

(P38 (W) KINASE)

L10 0 L9 AND P38 KINASE

=> s 19 and kinase inhibitors

266776 KINASE

52258 KINASES

275331 KINASE

(KINASE OR KINASES)

518345 INHIBITORS

20896 KINASE INHIBITORS

(KINASE(W) INHIBITORS)

L11 1 L9 AND KINASE INHIBITORS

=> s l9 and us/pc

1557202 US/PC

L12 11 L9 AND US/PC

=> d his

(FILE 'HOME' ENTERED AT 11:58:23 ON 25 JUN 2006)

FILE 'REGISTRY' ENTERED AT 11:58:36 ON 25 JUN 2006

L1 STRUCTURE UPLOADED

L2 1 S L1

L3 3 S L1 SSS FULL

L4 STRUCTURE UPLOADED

L5 11 S L4

L6 170 S L4 SSS FULL

FILE 'HCAPLUS' ENTERED AT 12:00:18 ON 25 JUN 2006

L7 2 S L3

L8 35 S L6

L9 28 S L8 AND PY<=2003

L10 0 S L9 AND P38 KINASE

L11 1 S L9 AND KINASE INHIBITORS

L12 11 S L9 AND US/PC

=> d l7 ibib abs hitstr tot

L7 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2006 ACS ON STN

ACCESSION NUMBER: 2004:878161 HCAPLUS

DOCUMENT NUMBER: 141:366245

TITLE: Preparation of substituted quinazolines as p38 kinase inhibitors

INVENTOR(S): Dunn, James Patrick; Goldstein, David Michael; Stahl, Christoph Martin; Trejo-Martin, Teresa Alejandra

PATENT ASSIGNEE(S): E. Hoffmann-La Roche AG, USA

SOURCE: U.S. Pat. Appl. Publ., 20 pp.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2004209904	A1	20041021	US 2004-824731	20040415
AU 2004230209	A1	20041028	AU 2004-230209	20040408
CA 2522522	AA	20041028	CA 2004-2522522	20040408
WO 2004092144	A2	20041028	WO 2004-EP3779	20040408
WO 2004092144	A3	20050324		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE,

ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI,
SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN,
TD, TG

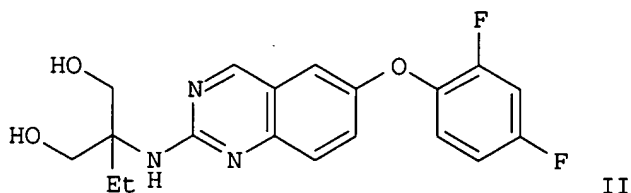
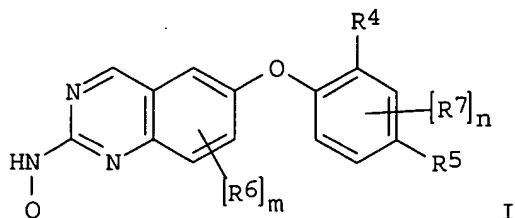
EP 1620408 A2 20060201 EP 2004-726448 20040408
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK

BR 2004009580 A 20060418 BR 2004-9580 20040408
CN 1774425 A 20060517 CN 2004-80010341 20040408

PRIORITY APPLN. INFO.:

US 2003-463467P P 20030416
WO 2004-EP3779 W 20040408

OTHER SOURCE(S): MARPAT 141:366245
GI



AB The title compds. I [R4, R5 = H, halo, CN, haloalkyl, or haloalkoxy (but are not both hydrogen); R6, R7 = alkyl, halo, CN, etc.; Q = a non-aromatic moiety; m = 0-3; n = 0-2] which are useful as p38 kinase inhibitors, were prepared and formulated. E.g., a multi-step synthesis of II, starting from Me 5-chloro-2-nitrobenzoate and 2,4-difluorophenol, which showed IC50 of <0.10 μ M against p38 MAP kinase, was given.

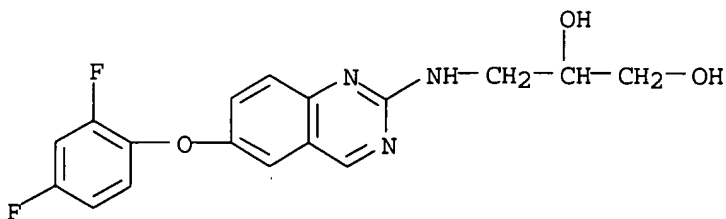
IT **778639-20-6P 778639-21-7P**

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

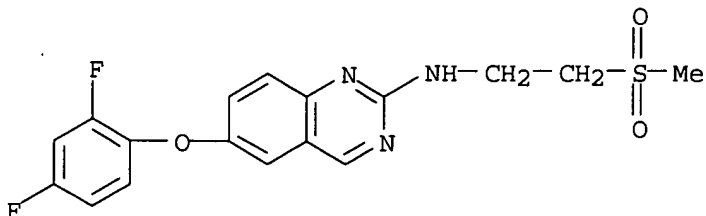
(preparation of substituted quinazolines as p38 kinase inhibitors)

RN 778639-20-6 HCAPLUS

CN 1,2-Propanediol, 3-[[6-(2,4-difluorophenoxy)-2-quinazolinyl]amino] - (9CI)
(CA INDEX NAME)



RN 778639-21-7 HCAPLUS
 CN 2-Quinazolinamine, 6-(2,4-difluorophenoxy)-N-[2-(methylsulfonyl)ethyl]-
 (9CI) (CA INDEX NAME)



L7 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 2004:582372 HCAPLUS
 DOCUMENT NUMBER: 142:155900
 TITLE: Synthesis and phenotypic screening of a
 guanine-mimetic library
 AUTHOR(S): Miller, Stephen C.; Mitchison, Timothy J.
 CORPORATE SOURCE: Department of Cell Biology and Institute of Chemistry
 and Cell Biology, Harvard Medical School, Boston, MA,
 02115, USA
 SOURCE: ChemBioChem (2004) 5(7), 1010-1012
 CODEN: CBCHFX ISSN: 1439-4227
 PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 142:155900
 GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Guanine-derived small mols. play important roles in many aspects of cellular function. Proteins that bind guanine and its derivs. control a wide variety of cellular processes, and compds. that disrupt this binding would be valuable research tools as well as potential pharmaceuticals. A split-pool library of 270 6-substituted-2-amino-4(3H)-quinazolinones (I) (R1 = residue of thiol, phenol, or primary alcs.; R2 = aryl or alkyl; e.g. R1 = 3,4-dimethylphenyl, R2 = 3,4,5-trimethoxyphenyl, benzyl; R1 = isobutylthio, R2 = 3-acetylphenyl; R1 = cyclohexylthio, R2 = 4-chlorophenyl) was prepared by aza-Wittig-mediated solid-phase synthesis which involves (1) nucleophilic aromatic substitution of a resin-bound 5-fluoro-2-nitrobenzamide with a variety of thiols, phenols, and primary alcs., (2) generation of a resin-bound iminophosphorane (II) (P = resin) by treatment with Ph3P/Cl3CCCl3/imidazole (3 h, 4°), (3) aza-Wittig reaction of the iminophosphoranes with one of 15 isocyanates (R2-NCO) to yield a carbodiimide (III) (P = resin) followed by intermol. O-attack instead of the desired N attack to the carbodiimide to yield an 4-imino-4H-3,1-benzoxazine (IV), and (4) DBU-mediated isomerization to the desired 2-amino-4(3H)-quinazolinone (V) (P = resin) followed by resin cleavage. The compds. I were cell-permeable guanine-mimetics and screened for (a) the effect on the cytoskeleton and cell cycle progression by incubating the compds. with BS-C-1-(monkey) cells for 6 h, followed by

fixing and staining for actin, DNA, and microtubules and (b) disruption of cellular trafficking. For example, I (R1 = isobutylthio, R2 = 3-acetylphenyl) disrupted both the actin and microtubule cytoskeleton, but did not arrest cells in mitosis.

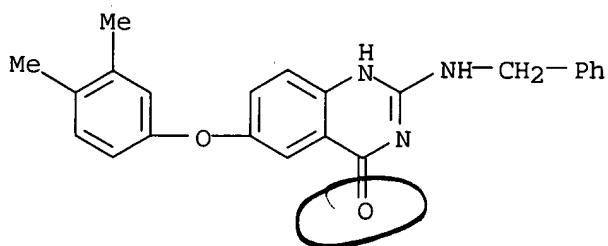
IT 828261-87-6P

RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(solid-phase synthesis and phenotypic screening of guanine-mimetic library via aza-Wittig reaction of iminophosphoranes with isocyanates and DBU-mediated isomerization iminobenzoxazines)

RN 828261-87-6 HCAPLUS

CN 4(1H)-Quinazolinone, 6-(3,4-dimethylphenoxy)-2-[(phenylmethyl)amino]-(9CI) (CA INDEX NAME)



REFERENCE COUNT:

9

THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d l11 ibib abs hitstr tot

L11 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1997:568090 HCAPLUS

DOCUMENT NUMBER: 127:248122

TITLE: Quinazoline derivatives as antitumor agents

INVENTOR(S): Barker, Andrew John; Johnstone, Craig

PATENT ASSIGNEE(S): Zeneca Limited, UK

SOURCE: PCT Int. Appl., 77 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9730034	A1	19970821	WO 1997-GB344	19970210 <--
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, UZ, VN, YU				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
CA 2242102	AA	19970821	CA 1997-2242102	19970210 <--
AU 9716126	A1	19970902	AU 1997-16126	19970210 <--
AU 707339	B2	19990708		
EP 880507	A1	19981202	EP 1997-902496	19970210 <--
EP 880507	B1	20050413		

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
IE, FI

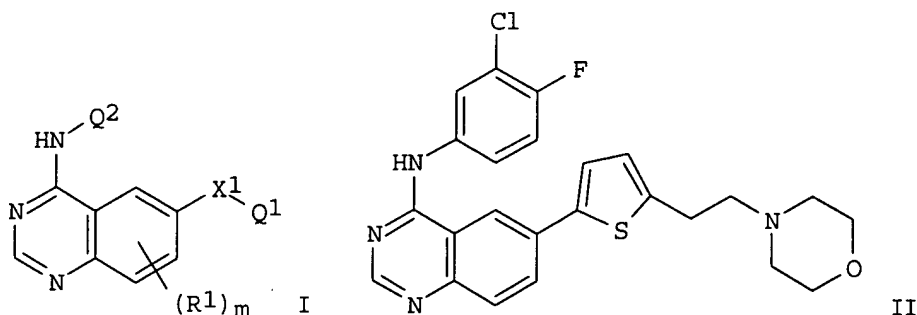
CN 1211240 A 19990317 CN 1997-192242 19970210 <--
 JP 2000504713 T2 20000418 JP 1997-529073 19970210 <--
 NZ 330816 A 20000526 NZ 1997-330816 19970210 <--
 IL 125685 A1 20021110 IL 1997-125685 19970210 <--
 AT 293103 E 20050415 AT 1997-902496 19970210
 PT 880507 T 20050729 PT 1997-902496 19970210
 ES 2239351 T3 20050916 ES 1997-902496 19970210
 ZA 9701231 A 19970814 ZA 1997-1231 19970213 <--
 US 5866572 A 19990202 US 1997-796483 19970213 <--
 NO 9803707 A 19981013 NO 1998-3707 19980813 <--
 NO 311936 B1 20020218
 US 6399602 B1 20020604 US 1998-152070 19980911 <--
 US 2003018029 A1 20030123 US 2002-136276 20020502 <--
 US 6897214 B2 20050524

PRIORITY APPLN. INFO.:

GB 1996-3095 A 19960214
 WO 1997-GB344 W 19970210
 US 1997-796483 A3 19970213
 US 1998-152070 A1 19980911

OTHER SOURCE(S):
GI

MARPAT 127:248122



AB The invention concerns quinazoline derivs. I [X^1 = bond, CO, $C(R^2)_2$, $CH(OR^2)$, S, C.tplbond.C, O, S, etc.; Q^1 = Ph, naphthyl, or 5- or 6-membered heteroaryl optionally bearing 1-3 substituents; m = 1 or 2; R^1 = H, halo, CF_3 , OH, NH_2 , cyano, etc.; R^2 = H, alkyl; Q^2 = Ph or 9- or 10-membered bicyclic heterocycle optionally bearing 1-3 substituents] and their pharmaceutically acceptable salts. Also disclosed are processes for preparation of I and salts, pharmaceutical compns. containing them, and the use of

their receptor tyrosine kinase inhibitory properties in the treatment of proliferative diseases such as cancer. Examples include syntheses of 40 compds. and various intermediates. For instance, $Pd(PPh_3)_4$ -catalyzed coupling of 6-bromo-4-(3-chloro-4-fluoroanilino)quinazoline-HCl with di-iso-Pr [5-(2-morpholinoethyl)thien-2-yl]boronate (prepn. given) gave 27% title compound II. At 50 mg/kg/day in athymic nude mice with human vulval epidermoid carcinoma xenografts (cell line A-431), II gave 64% inhibition of tumor volume (vs. control) after 13 days.

IT **195457-37-5P**, 4-(3-Chloro-4-fluoroanilino)-6-(4-cyanophenoxy)quinazoline **195457-38-6P**, 4-(3-Chloro-4-fluoroanilino)-6-(4-nitrophenoxy)quinazoline **195457-39-7P**, 6-(4-Aminophenoxy)-4-(3-chloro-4-fluoroanilino)quinazoline **195457-41-1P**, 6-[4-(Aminomethyl)phenoxy]-4-(3-chloro-4-

06/25/2006

10824731.trn

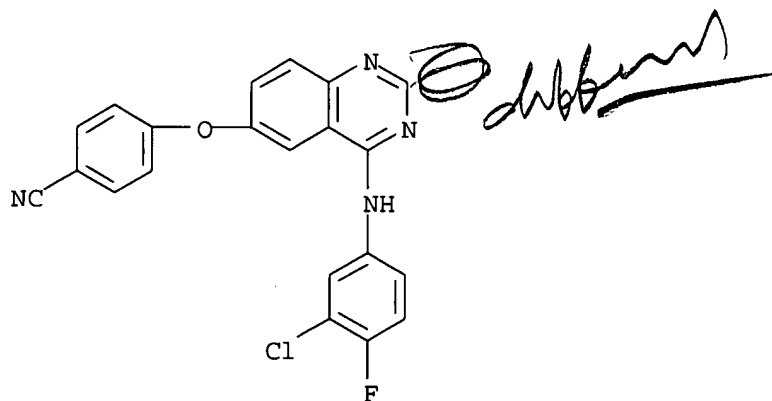
fluoroanilino)quinazoline

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of quinazoline derivs. as antitumor agents and antiproliferatives)

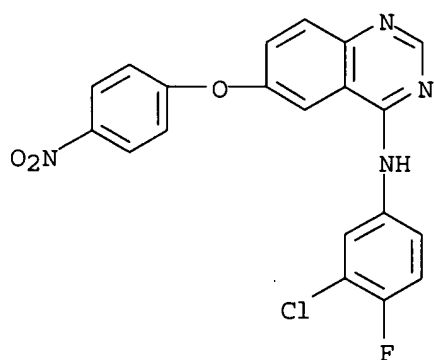
RN 195457-37-5 HCAPLUS

CN Benzonitrile, 4-[[4-[(3-chloro-4-fluorophenyl)amino]-6-quinazolinyl]oxy]-(9CI) (CA INDEX NAME)



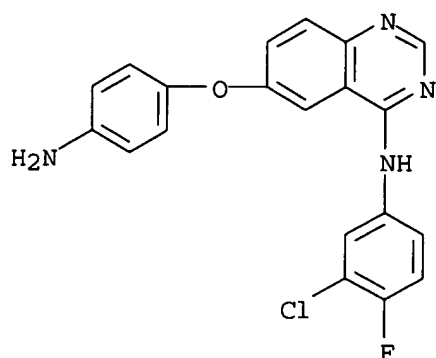
RN 195457-38-6 HCAPLUS

CN 4-Quinazolinamine, N-(3-chloro-4-fluorophenyl)-6-(4-nitrophenoxy)-(9CI) (CA INDEX NAME)



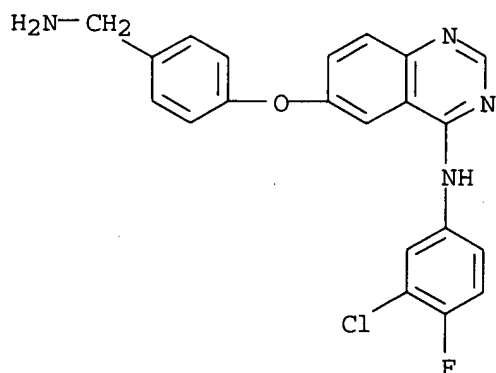
RN 195457-39-7 HCAPLUS

CN 4-Quinazolinamine, 6-(4-aminophenoxy)-N-(3-chloro-4-fluorophenyl)-(9CI) (CA INDEX NAME)



RN 195457-41-1 HCAPLUS

CN 4-Quinazolinamine, 6-[4-(aminomethyl)phenoxy]-N-(3-chloro-4-fluorophenyl)-
(9CI) (CA INDEX NAME)



IT 195457-40-0P, 4-(3-Chloro-4-fluoroanilino)-6-phenoxyquinazoline

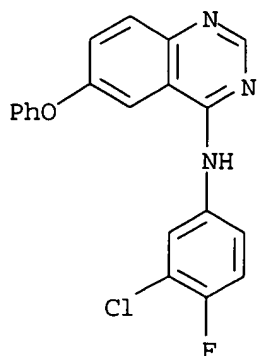
195457-42-2P, 4-(3-Chloro-4-fluoroanilino)-6-[4-(morpholinomethyl)phenoxy]quinazoline

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

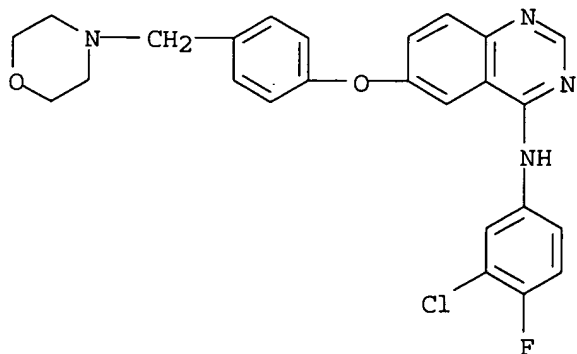
(preparation of quinazoline derivs. as antitumor agents and antiproliferatives)

RN 195457-40-0 HCAPLUS

CN 4-Quinazolinamine, N-(3-chloro-4-fluorophenyl)-6-phenoxy- (9CI) (CA INDEX NAME)



RN 195457-42-2 HCAPLUS
 CN 4-Quinazolinamine, N-(3-chloro-4-fluorophenyl)-6-[4-(4-morpholinylmethyl)phenoxy]-(9CI) (CA INDEX NAME)



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L12 ANSWER 1 OF 11 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2003:737351 HCAPLUS

DOCUMENT NUMBER: 139:261565

TITLE: Preparation of quinazolinylguanidines, quinolinylguanidines, and N-sulfonyl argininyphenylalaninamides for the treatment of pain
 INVENTOR(S): Forray, Carlos C.; Kawakami, Joel; Konkell, Michael J.; Boteju, Lakmal W.; Wetzel, John M.; Noble, Stewart A.; Wan, Honghe

PATENT ASSIGNEE(S): USA

SOURCE: U.S. Pat. Appl. Publ., 47 pp.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2003176314	A1	20030918	US 2002-253237	20020924 <--
PRIORITY APPLN. INFO.:			US 2001-324767P	P 20010924

AB Title compds. were prepared for treating pain, urinary incontinence and other abnormalities mediated by a neuropeptide FF (NPFF) receptor. Thus, N-(4-methyl-6-pentyl-2-quinazolinyl)guanidine and 1-naphthalenesulfonyl-Arg-Phe-NH₂ were prepared and shown to be agonists concurrently at the NPFF1 and NPFF2 receptors.

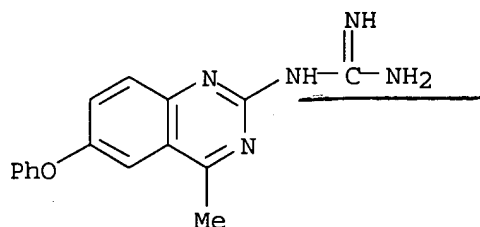
IT 503831-93-4P 503831-96-7P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of quinazolinylguanidines, quinolinyguanidines, and N-sulfonyl argininyphenylalaninamides for treatment of pain)

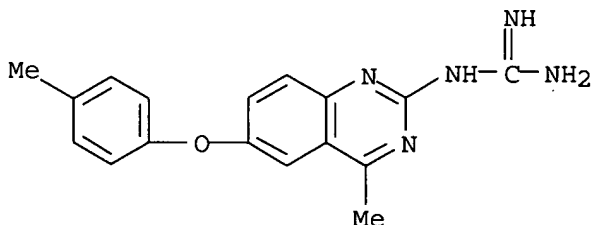
RN 503831-93-4 HCAPLUS

CN Guanidine, (4-methyl-6-phenoxy-2-quinazolinyl)- (9CI) (CA INDEX NAME)



RN 503831-96-7 HCAPLUS

CN Guanidine, [4-methyl-6-(4-methylphenoxy)-2-quinazolinyl]- (9CI) (CA INDEX NAME)



L12 ANSWER 2 OF 11 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2003:570646 HCAPLUS

DOCUMENT NUMBER: 139:133576

TITLE: Preparation of quinolyl- and quinazolinylguanidines as neuropeptide FF (NPFF) agonists/antagonists for treatment of urge incontinence.

INVENTOR(S): Kawakami, Joel K.; Wetzel, John; Boteju, Lakmal W.; Konkell, Michael J.; Wan, Honghe; Noble, Stewart A.

PATENT ASSIGNEE(S): USA

SOURCE: U.S. Pat. Appl. Publ., 52 pp.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

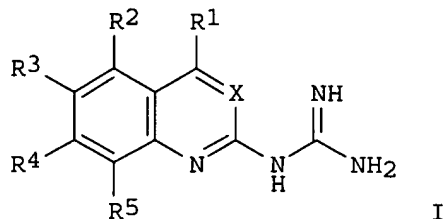
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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US 2003139431
 PRIORITY APPLN. INFO.:
 OTHER SOURCE(S):
 GI

A1 20030724
 MARPAT 139:133576

US 2002-253946
 US 2001-324559P

20020921 <--
 P 20010924



AB A method for treating urge incontinence comprises administration of title compds. [I; X = CH, CMe, N; R1-R5 = H, alkyl, alkenyl, alkynyl, cycloalkyl, (substituted) aryl, OH, halogenated ether, NO2, amino, halo, CN, C(Z)R6, C(Z)OR6, C(Z)N(R6)2, N(R6)C(Z)R6, N(R6)C(Z)N(R6)2, OC(Z)R6, C(Z)OR6, OR6, SR6; Z = O, S; R6 = alkyl, aryl, (CH2)nQ, alkenyl, cycloalkyl, cycloalkenyl, Q = OR7, SR7, N(R7)2, aryl; R7 = H, alkyl, alkenyl, alkynyl, cycloalkyl, cycloalkenyl, aryl; R2R3 = fused aryl, heteroaryl, cycloalkyl, heterocyclic alkyl ring; R3R4 = fused aryl, heteroaryl, cycloalkyl, heterocyclic alkyl ring; each alkyl, alkenyl, alkynyl, alkoxy group is optionally substituted with Ra; Ra = OH, alkoxy, halo, NO2, amino, CF3, carboxy; each cycloalkyl group is optionally substituted with Rb; Rb = Ra, alkyl, alkenyl, alkynyl, cycloalkyl; each aryl is optionally substituted with R1]. Thus, I (X = CH; R1 = Me; R2, R4, R5 = H; R3 = Cl) at 1 mg/kg i.v. in female rats produced complete inhibition of distention-induced bladder contractions, resulting in a disappearance time of 35 min.

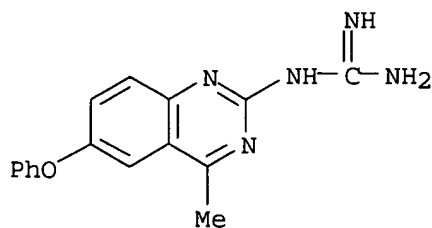
IT 503831-93-4P, N-(4-Methyl-6-phenoxy-2-quinazolinyl)guanidine
 503831-96-7P, N-[4-Methyl-6-(4-methylphenoxy)-2-quinazolinyl]guanidine

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of quinolylguanidines and quinazolinylguanidines as neuropeptide FF (NPFF) agonists/antagonists for treatment of urge incontinence)

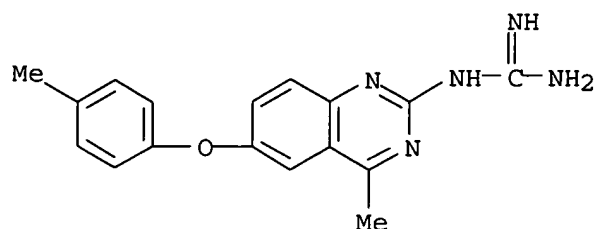
RN 503831-93-4 HCAPLUS

CN Guanidine, (4-methyl-6-phenoxy-2-quinazolinyl)- (9CI) (CA INDEX NAME)



RN 503831-96-7 HCAPLUS

CN Guanidine, [4-methyl-6-(4-methylphenoxy)-2-quinazolinyl]- (9CI) (CA INDEX NAME)



L12 ANSWER 3 OF 11 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2003:335019 HCAPLUS

DOCUMENT NUMBER: 138:346575

TITLE: Imide compounds and their application in optical recording media

INVENTOR(S): Ogiso, Akira; Shiozaki, Hiroyoshi; Ishida, Tsutomu; Tsukahara, Hisashi; Misawa, Tsutami; Inoue, Koji; Koike, Tadashi; Ueno, Keiji; Inatomi, Yuji; Nara, Ryousuke

PATENT ASSIGNEE(S): Mitsui Chemicals, Inc., Japan

SOURCE: PCT Int. Appl., 205 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003035407	A1	20030501	WO 2002-JP10939	20021022 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1445115	A1	20040811	EP 2002-777915	20021022
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
CN 1575236	A	20050202	CN 2002-820890	20021022
JP 2004042596	A2	20040212	JP 2002-324789	20021108
US 2005208425	A1	20050922	US 2004-493034	20040419 <--
PRIORITY APPLN. INFO.:				
			JP 2001-323900	A 20011022
			JP 2001-344742	A 20011109
			JP 2002-147538	A 20020522
			JP 2002-210949	A 20020719
			JP 2002-244776	A 20020826
			JP 2002-246872	A 20020827
			WO 2002-JP10939	W 20021022

OTHER SOURCE(S): MARPAT 138:346575

AB An optical recording medium contains in its recording layer at least one imide compound having a metallocene substitution group.

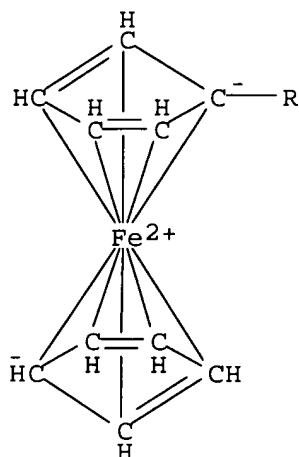
IT 516516-47-5 516517-77-4 516518-99-3

RL: MOA (Modifier or additive use); USES (Uses)
(metallocene-containing imide compds. optical recording media)

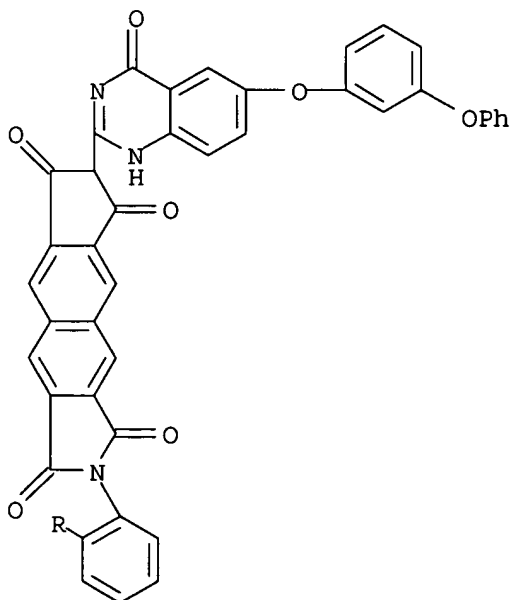
RN 516516-47-5 HCAPLUS

CN Ferrocene, [2-[7-[1,4-dihydro-4-oxo-6-(3-phenoxyphenoxy)-2-quinazolinyl]-3,6,7,8-tetrahydro-1,3,6,8-tetraoxoindeno[5,6-f]isoindol-2(1H)-yl]phenyl]-(9CI) (CA INDEX NAME)

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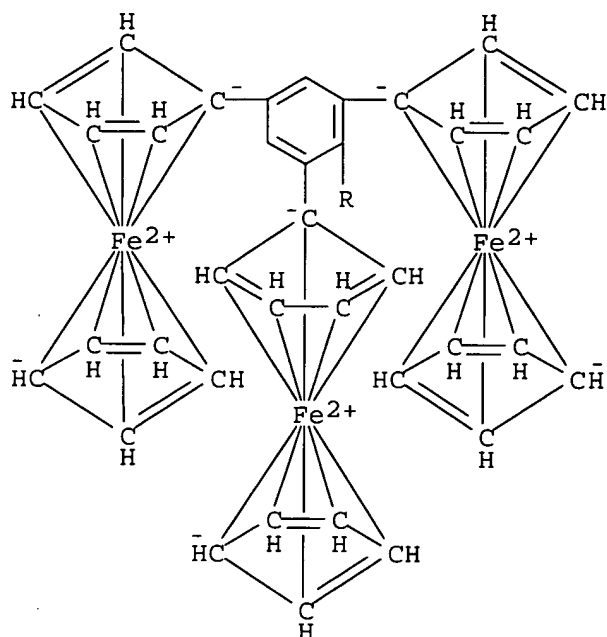
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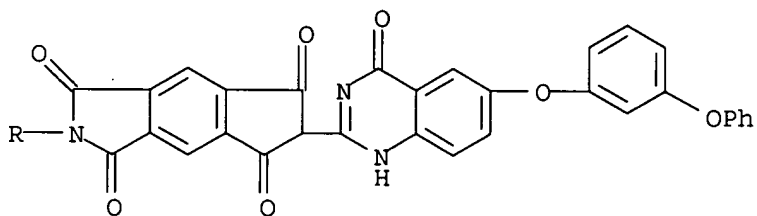
RN 516517-77-4 HCAPLUS

CN Ferrocene, 1,1',1''-[2-[6-[1,4-dihydro-4-oxo-6-(3-phenoxyphenoxy)-2-quinazolinyl]-3,5,6,7-tetrahydro-1,3,5,7-tetraoxocyclopent[f]isoindol-2(1H)-yl]-1,3,5-benzenetriyl]tris- (9CI) (CA INDEX NAME)

PAGE 1-A



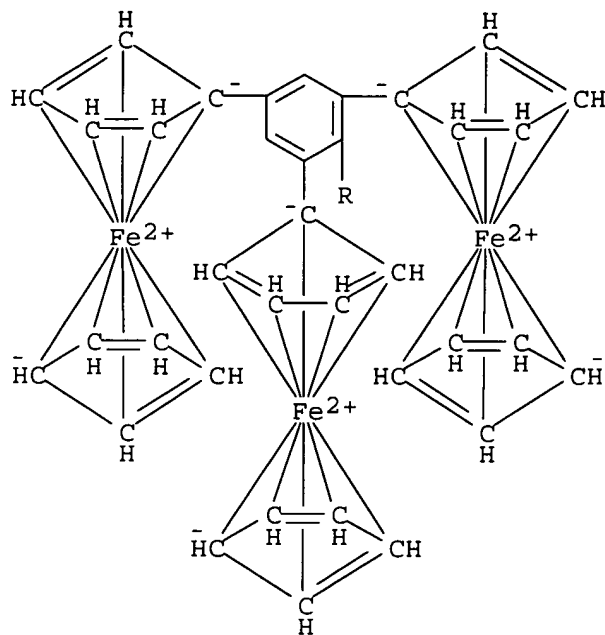
PAGE 2-A



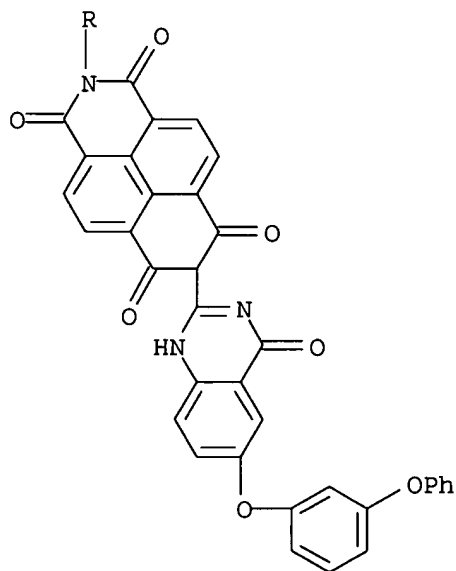
RN 516518-99-3 HCAPLUS

CN Ferrocene, 1,1',1''',1''''-[2-[7-[1,4-dihydro-4-oxo-6-(3-phenoxyphenoxy)-2-quinazolinyl]-3,6,7,8-tetrahydro-1,3,6,8-tetraoxonaphth[2,1,8-def]isoquinolin-2(1H)-yl]-1,3,5-benzenetriyl]tris- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



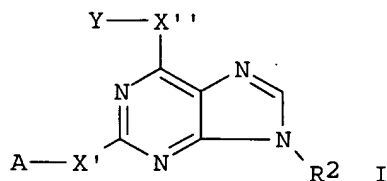
REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 4 OF 11 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:301049 HCAPLUS
DOCUMENT NUMBER: 138:321058
TITLE: C2-, C6- and 9-Aryl-substituted purine and other

heteroaryl kinase inhibitor scaffolds and methods for their preparation

INVENTOR(S): Ding, Sheng; Ding, Qiang; Gray, Nathanael S.
 PATENT ASSIGNEE(S): IRM LLC, Bermuda
 SOURCE: PCT Int. Appl., 68 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003031406	A2	20030417	WO 2002-US32680	20021012 <--
WO 2003031406	A3	20060105		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2463563	AA	20030417	CA 2002-2463563	20021012 <--
US 2003191312	A1	20031009	US 2002-270030	20021012 <--
JP 2005512972	T2	20050512	JP 2003-534390	20021012
EP 1578722	A2	20050928	EP 2002-776216	20021012
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
US 2006009642	A1	20060112	US 2005-223429	20050909 <--
PRIORITY APPLN. INFO.:				
			US 2001-328763P	P 20011012
			US 2001-331835P	P 20011120
			US 2002-346480P	P 20020107
			US 2002-348089P	P 20020110
			US 2001-328741P	P 20011012
			US 2002-346552P	P 20020107
			US 2002-347037P	P 20020108
			US 2002-170031	A3 20020612
			WO 2002-US32680	W 20021012
OTHER SOURCE(S): CASREACT 138:321058; MARPAT 138:321058				
GI				



AB General methods for the solution phase as well as solid phase synthesis of various substituted heteroaryls, particularly C2-, C6- and 9-aryl-substituted purines (e.g. 2-(2,4-dimethoxyphenyl)-6-(4-methoxybenzylamino)-9-isopropylpurine), was demonstrated. These substituted heteroaryls can be further elaborated by aromatic substitution

with amines at elevated temperature or by anilines, boronic acids and phenols via Pd catalyzed cross-coupling reactions. The 1st claim comprises a method of preparing a C2-substituted purine compound, said method comprising: reacting a C2-halogenated purine with A-X (X = -B(OH)₂, -OH, and -NHR₁; R₁ = H, (un)substituted alkyl; A = (un)substituted alkyl, (un)substituted aryl, (un)substituted heterocyclyl) in the presence of a solvent, a base, a carbene ligand and a Pd catalyst. The 2nd claims narrows the 1st claim to purines I wherein R₂ = H, (un)substituted alkyl, (un)substituted aryl, (un)substituted heterocyclyl; X' = direct bond, NR₁ and O; X'' = direct bond, O and NR₃, with the proviso that when X'' is NR₃, Y is R₄ or A', and when X' is O or a direct bond, Y is A'; A' = (un)substituted alkyl, (un)substituted aryl, (un)substituted arylalkyl, (un)substituted heterocyclyl; R₃ = H, (un)substituted alkyl; and R₄ = (un)substituted alkyl. Similar claims pertain to C6-substituted purines. Also claimed is a method of preparing a 9-aryl substituted purines, the method comprising: reacting a 2,6-dihalogenated purine with Ar-B(OH)₂ (Ar = (un)substituted aryl, and (un)substituted heterocyclyl) in the presence of a solvent and a Cu catalyst. Also claimed is a method for synthesizing a substituted heteroaryl, the method comprising: providing a dihaloheteroaryl scaffold moiety and capturing the dihaloheteroaryl scaffold moiety on a resin by nucleophilic substitution of a 1st halogen by a resin-bound amine nucleophile to afford a resin-bound amine substituted monohaloheteroaryl. Substitution of the 2nd halogen is done by nucleophilic displacement (e.g. by aniline, phenol, amine, boronic acid) or coupling (e.g. palladium-mediated). An initial substitution (e.g. alkylation, acylation, coupling) can be done prior to substitution of the 1st halogen. Example procedures are included for: boronic acid coupling, aniline coupling, phenol coupling, purine N9 arylation via boronic acids/cupric acetate, reductive amination for synthesis of PAL-resin-bound amine, resin capture of dichloroheterocycles, substitution of remaining chloro group with boronic acids via Suzuki coupling and product cleavage, substitution of remaining chloro group with anilines or amines via palladium-catalyzed reaction and product cleavage, substitution of remaining chloro group with phenols via palladium-catalyzed reaction and product cleavage, substitution of remaining chloro group with amines via non-palladium-catalyzed amination reaction without base and product cleavage, and substitution of remaining chloro group with amines via non-palladium-catalyzed amination reaction with K⁺OT⁻Bu as base and product cleavage. Tables of purity and yields for various heteroaryl combinatorial libraries are included as validation of the following methods: palladium catalyzed cross-coupling reactions for derivatizing resin-bound 2-chloro-6-aminopurine with boronic acids, anilines, amines and phenols, resin-bound chloroheterocyclic scaffolds which can be derivatized via Suzuki coupling reaction, resin-bound chloroheterocyclic scaffolds which can be derivatized via palladium catalyzed amination reaction, and resin-bound chloroheterocyclic scaffolds which can be derivatized via palladium catalyzed C-O bond formation reaction.

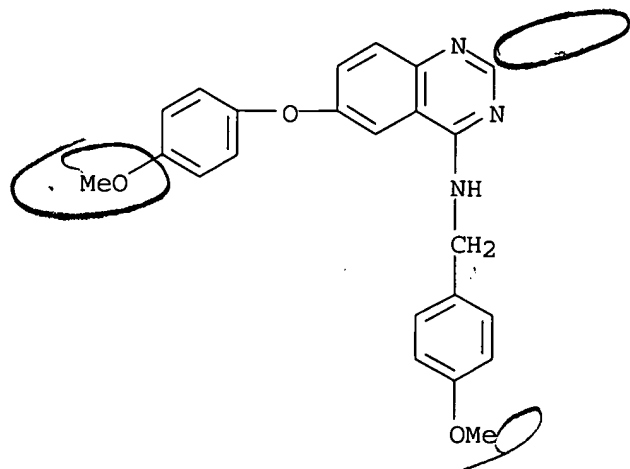
IT **406932-80-7P**, 4-(4-Methoxybenzylamino)-6-(4-methoxyphenoxy)quinazoline

RL: CPN (Combinatorial preparation); CMBI (Combinatorial study); PREP (Preparation)

(C2-, C6- and 9-Aryl-substituted purine and other heteroaryl kinase inhibitor scaffolds and methods for their preparation)

RN 406932-80-7. HCAPLUS

CN 4-Quinazolinamine, 6-(4-methoxyphenoxy)-N-[(4-methoxyphenyl)methyl]- (9CI)
(CA INDEX NAME)



L12 ANSWER 5 OF 11 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2002:171851 HCAPLUS

DOCUMENT NUMBER: 136:232110

TITLE: Preparation of phenoxybenzylamines as selective serotonin re-uptake inhibitors

INVENTOR(S): Adam, Mavis Diane; Andrews, Mark David; Elliott, Mark Leonard; Gymer, Geoffrey Edward; Hepworth, David; Howard, Harry Ralph, Jr.; Middleton, Donald Stuart; Stobie, Alan

PATENT ASSIGNEE(S): Pfizer Limited, UK; Pfizer Inc.

SOURCE: PCT Int. Appl., 110 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

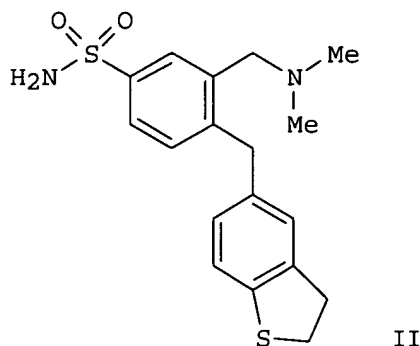
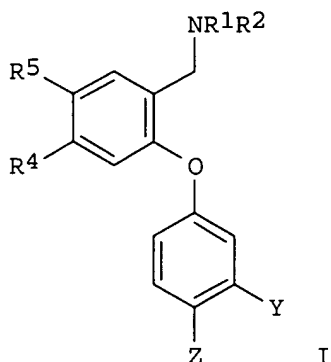
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002018333	A1	20020307	WO 2001-IB1521	20010822 <--
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
CA 2420969	AA	20020307	CA 2001-2420969	20010822 <--
AU 2001078650	A5	20020313	AU 2001-78650	20010822 <--
EP 1313701	A1	20030528	EP 2001-956734	20010822 <--
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR			
BR 2001013610	A	20030624	BR 2001-13610	20010822 <--
JP 2004507523	T2	20040311	JP 2002-523451	20010822
NZ 523951	A	20040924	NZ 2001-523951	20010822
EE 200300084	A	20050215	EE 2003-84	20010822
US 2003060456	A1	20030327	US 2001-941177	20010827 <--
US 6610747	B2	20030826		
BG 107544	A	20031031	BG 2003-107544	20030207 <--

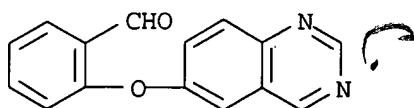
ZA 2003001383	A	20040402	ZA 2003-1383	20030220
NO 2003000842	A	20030428	NO 2003-842	20030224 <--
HR 2003000141	A1	20030430	HR 2003-141	20030226 <--
PRIORITY APPLN. INFO.:			GB 2000-21593	A 20000831
			GB 2001-7116	A 20010321
			US 2000-240271P	P 20001013
			US 2001-292400P	P 20010521
			WO 2001-IB1521	W 20010822

OTHER SOURCE(S): MARPAT 136:232110
GI



AB Title compds. I [R¹ and R² independently = H, alkyl or (CH₂)_n(C₃-C₆cycloalkyl) wherein n = 0, 1, 2 or 3; or R¹ and R² together with the nitrogen to which they are attached from an azetidine ring; Z or Y is -SR³ and the other Z or Y is halogen or -R³; wherein R³ = C₁-4 alkyl optionally substituted with fluorine; except that R³ is not CF₃; or Z and Y are linked so that, together with the interconnecting atoms, Z and Y form a fused 5 to 7-membered carbocyclic or heterocyclic ring, and wherein when Z and Y form a heterocyclic ring, in addition to carbon atoms, the linkage contains one or two heteroatoms independently selected from O, S and N; R⁴ and R⁵ independently = A-X, wherein A = -CH=CH- or -(CH₂)_p- where p is 0, 1 or 2; X = H, halo, CONR⁶R⁷, SO₂NR⁶R⁷, SO₂NHC(=O)R⁶, OH, C₁-4alkoxy, etc; or A-X = (un)substituted 5- or 6-membered heterocyclic ring containing 1, 2 or 3 heteroatoms selected from N, S and O; R⁶ and R⁷ independently = H, (un)substituted alkyl; or R⁶ and R⁷ together with the N to which they are attached form a (un)substituted 4-6 membered heterocyclic ring] and there pharmaceutically acceptable salts are prepared. Thus, II was prepared via substitution of 5-(aminosulfonyl)-2-fluoro-N-methylbenzamide by 2,3-dihydrobenzo[b]thiophen-5-ol with successive BF₃·THF catalyzed amide reduction, formylation of secondary amine, and reduction. II demonstrated a serotonin re-uptake inhibition IC₅₀ of 4.7nM. I inhibit monoamine re-uptake and in particular exhibit activity as selective serotonin reuptake inhibitors.

IT 402911-71-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of serotonin re-uptake inhibitors phenoxybenzylamines)
RN 402911-71-1 HCAPLUS
CN Benzaldehyde, 2-(6-quinazolinylloxy)- (9CI) (CA INDEX NAME)



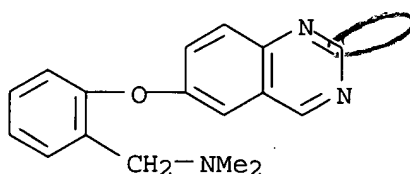
IT 402910-46-7P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(target compound; preparation of serotonin re-uptake inhibitors phenoxybenzylamines)

RN 402910-46-7 HCAPLUS

CN Benzenemethanamine, N,N-dimethyl-2-(6-quinazolin-2-yl)-, hydrochloride (9CI) (CA INDEX NAME)



● x HCl

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 6 OF 11 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1998:282401 HCAPLUS

DOCUMENT NUMBER: 128:321653

TITLE: Preparation of alkynyl- and azido-substituted 4-anilinoquinazolines for the treatment of hyperproliferative diseases

INVENTOR(S): Schnur, Rodney Caughren; Arnold, Lee Daniel

PATENT ASSIGNEE(S): Pfizer Inc., USA

SOURCE: U.S., 23 pp.

CODEN: USXXAM

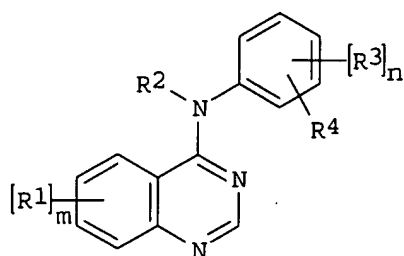
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5747498	A	19980505	US 1996-653786	19960528 <--
PRIORITY APPLN. INFO.:			US 1996-653786	19960528
OTHER SOURCE(S):		CASREACT 128:321653; MARPAT 128:321653		
GI				



AB The title compds. [I; R1 = H, halo, OH, etc.; R2 = H, (un)substituted C1-6 alkyl; R3 = H, halo, OH, etc.; R4 = N3, (un)substituted ethynyl; m = 1-3; n = 1-2] and their salts, useful in the treatment of hyperproliferative diseases such as cancer, were prepared Thus, reaction of 4-chloro-6,7-dimethoxyquinazoline with 4-azidoaniline hydrochloride in iPrOH afforded 98% I [R1 = 6,7-Me2; R2, R3 = H; R4 = 4-N3]. Compds. I showed IC50 of 0.0001-30 μ M against EGFR kinase.

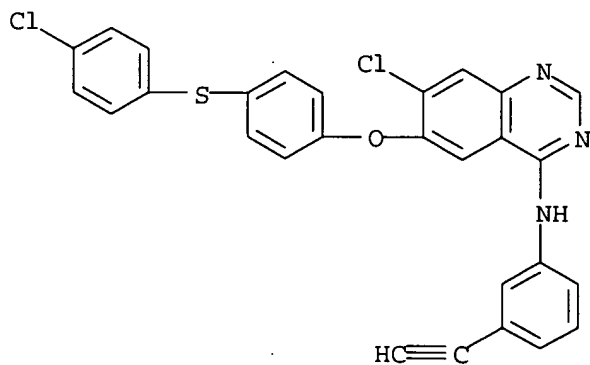
IT 207225-62-5P 207225-66-9P 207225-68-1P
 207225-69-2P 207225-70-5P 207225-77-2P
 207225-78-3P 207225-79-4P 207225-80-7P
 207225-81-8P 207225-82-9P 207225-83-0P
 207225-85-2P 207225-86-3P 207225-87-4P
 207225-89-6P 207225-90-9P 207225-92-1P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of alkynyl- and azido-substituted 4-anilinoquinazolines for the treatment of hyperproliferative diseases)

RN 207225-62-5 HCAPLUS

CN 4-Quinazolinamine, 7-chloro-6-[4-[(4-chlorophenyl)thio]phenoxy]-N-(3-ethynylphenyl)-, monohydrochloride (9CI) (CA INDEX NAME)



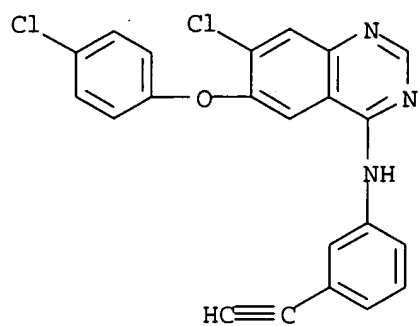
● HCl

RN 207225-66-9 HCAPLUS

CN 4-Quinazolinamine, 7-chloro-6-(4-chlorophenoxy)-N-(3-ethynylphenyl)-, monohydrochloride (9CI) (CA INDEX NAME)

06/25/2006

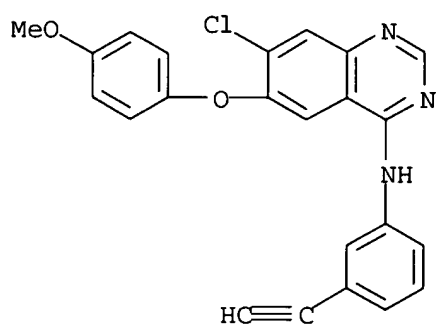
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● HCl

RN 207225-68-1 HCAPLUS

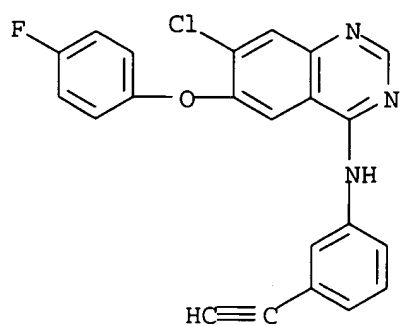
CN 4-Quinazolinamine, 7-chloro-N-(3-ethynylphenyl)-6-(4-methoxyphenoxy)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

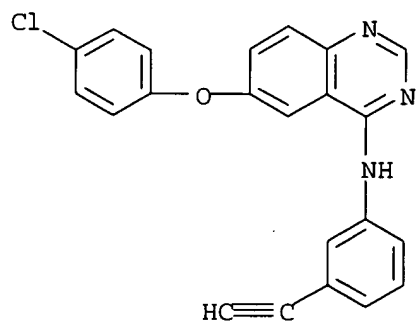
RN 207225-69-2 HCAPLUS

CN 4-Quinazolinamine, 7-chloro-N-(3-ethynylphenyl)-6-(4-fluorophenoxy)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 207225-70-5 HCAPLUS

CN 4-Quinazolinamine, 6-(4-chlorophenoxy)-N-(3-ethynylphenyl)-,
monohydrochloride (9CI) (CA INDEX NAME)

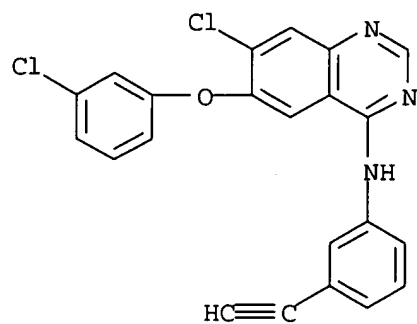
● HCl

RN 207225-77-2 HCAPLUS

CN 4-Quinazolinamine, 7-chloro-6-(3-chlorophenoxy)-N-(3-ethynylphenyl)-,
monohydrochloride (9CI) (CA INDEX NAME)

06/25/2006

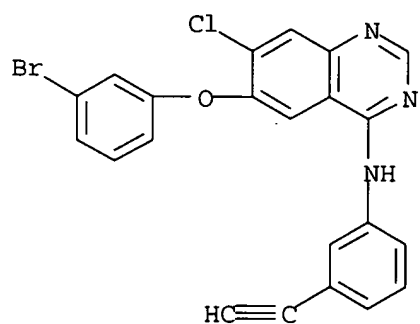
10824731.trn



● HCl

RN 207225-78-3 HCAPLUS

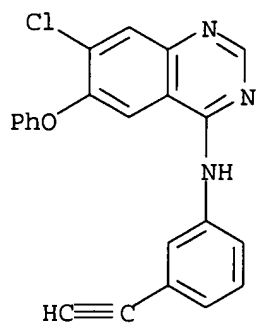
CN 4-Quinazolinamine, 6-(3-bromophenoxy)-7-chloro-N-(3-ethynylphenyl)-,
monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 207225-79-4 HCAPLUS

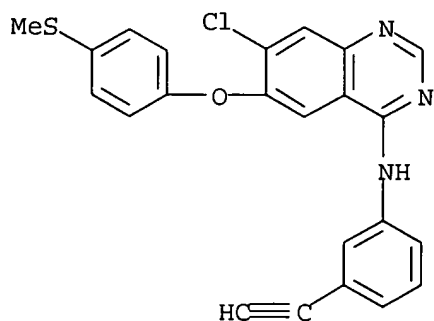
CN 4-Quinazolinamine, 7-chloro-N-(3-ethynylphenyl)-6-phenoxy-,
monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 207225-80-7 HCAPLUS

CN 4-Quinazolinamine, 7-chloro-N-(3-ethynylphenyl)-6-[4-(methylthio)phenoxy]-, monohydrochloride (9CI) (CA INDEX NAME)



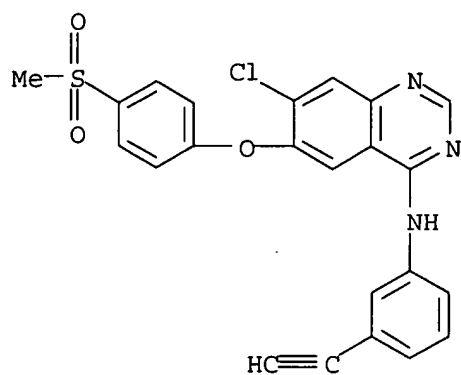
● HCl

RN 207225-81-8 HCAPLUS

CN 4-Quinazolinamine, 7-chloro-N-(3-ethynylphenyl)-6-[4-(methylsulfonyl)phenoxy]-, monohydrochloride (9CI) (CA INDEX NAME)

06/25/2006

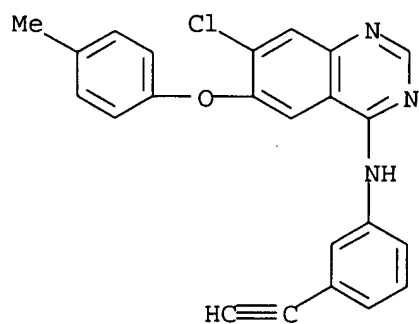
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● HCl

RN 207225-82-9 HCAPLUS

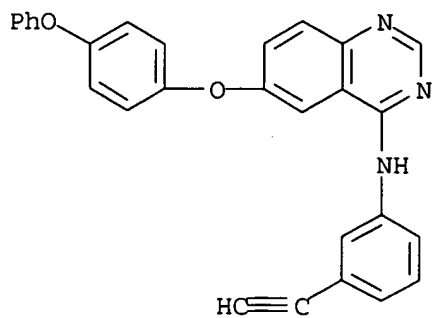
CN 4-Quinazolinamine, 7-chloro-N-(3-ethynylphenyl)-6-(4-methylphenoxy)-,
monohydrochloride (9CI) (CA INDEX NAME)



● HCl

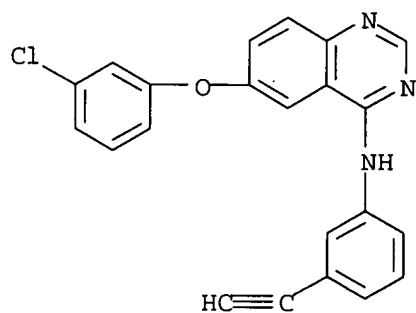
RN 207225-83-0 HCAPLUS

CN 4-Quinazolinamine, N-(3-ethynylphenyl)-6-(4-phenoxyphenoxy)-,
monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 207225-85-2 HCAPLUS

CN 4-Quinazolinamine, 6-(3-chlorophenoxy)-N-(3-ethynylphenyl)-,
monohydrochloride (9CI) (CA INDEX NAME)

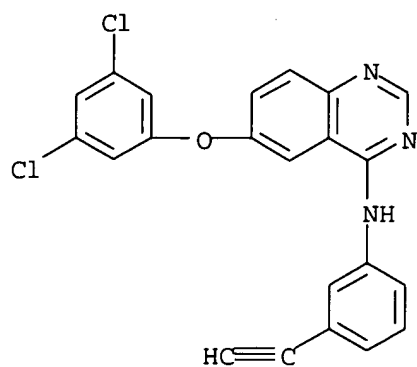
● HCl

RN 207225-86-3 HCAPLUS

CN 4-Quinazolinamine, 6-(3,5-dichlorophenoxy)-N-(3-ethynylphenyl)-,
monohydrochloride (9CI) (CA INDEX NAME)

06/25/2006

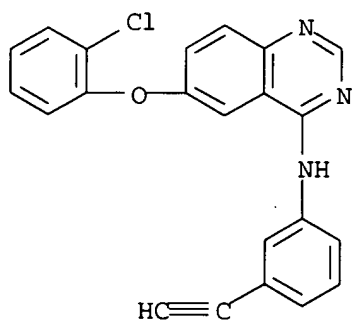
10824731.trn



● HCl

RN 207225-87-4 HCAPLUS

CN 4-Quinazolinamine, 6-(2-chlorophenoxy)-N-(3-ethynylphenyl)-,
monohydrochloride (9CI) (CA INDEX NAME)



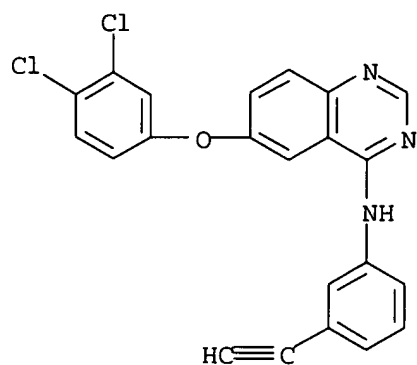
● HCl

RN 207225-89-6 HCAPLUS

CN 4-Quinazolinamine, 6-(3,4-dichlorophenoxy)-N-(3-ethynylphenyl)-,
monohydrochloride (9CI) (CA INDEX NAME)

06/25/2006

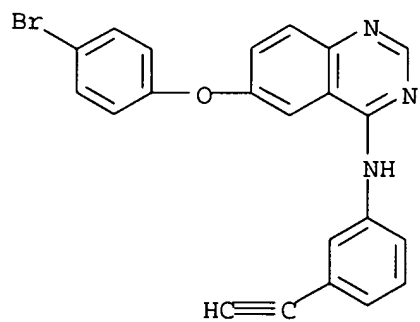
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● HCl

RN 207225-90-9 HCAPLUS

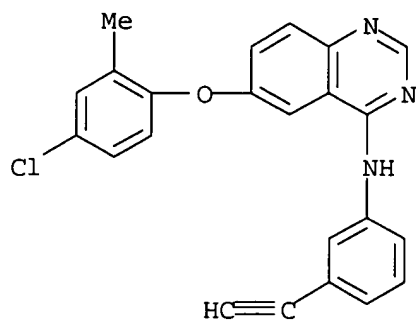
CN 4-Quinazolinamine, 6-(4-bromophenoxy)-N-(3-ethynylphenyl)-,
monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 207225-92-1 HCAPLUS

CN 4-Quinazolinamine, 6-(4-chloro-2-methylphenoxy)-N-(3-ethynylphenyl)-,
monohydrochloride (9CI) (CA INDEX NAME)



● HCl

REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 7 OF 11 HCAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 1997:568090 HCAPLUS
 DOCUMENT NUMBER: 127:248122
 TITLE: Quinazoline derivatives as antitumor agents
 INVENTOR(S): Barker, Andrew John; Johnstone, Craig
 PATENT ASSIGNEE(S): Zeneca Limited, UK
 SOURCE: PCT Int. Appl., 77 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9730034	A1	19970821	WO 1997-GB344	19970210 <--
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, UZ, VN, YU				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
CA 2242102	AA	19970821	CA 1997-2242102	19970210 <--
AU 9716126	A1	19970902	AU 1997-16126	19970210 <--
AU 707339	B2	19990708		
EP 880507	A1	19981202	EP 1997-902496	19970210 <--
EP 880507	B1	20050413		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
CN 1211240	A	19990317	CN 1997-192242	19970210 <--
JP 2000504713	T2	20000418	JP 1997-529073	19970210 <--
NZ 330816	A	20000526	NZ 1997-330816	19970210 <--
IL 125685	A1	20021110	IL 1997-125685	19970210 <--
AT 293103	E	20050415	AT 1997-902496	19970210
PT 880507	T	20050729	PT 1997-902496	19970210
ES 2239351	T3	20050916	ES 1997-902496	19970210
ZA 9701231	A	19970814	ZA 1997-1231	19970213 <--

06/25/2006

10824731.trn

US 5866572
NO 9803707
NO 311936
US 6399602
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US 6897214

A 19990202
A 19981013
B1 20020218
B1 20020604
A1 20030123
B2 20050524

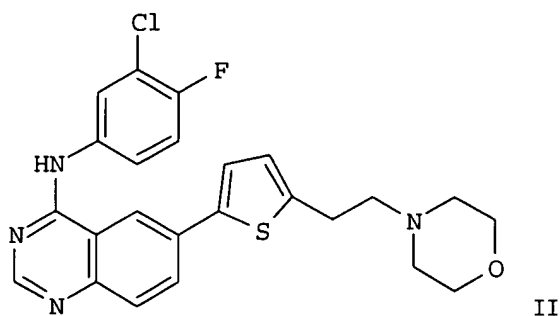
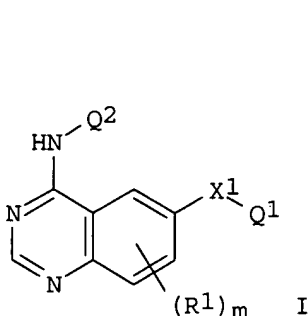
US 1997-796483
NO 1998-3707
US 1998-152070
US 2002-136276

19970213 <--
19980813 <--
19980911 <--
20020502 <--

PRIORITY APPLN. INFO.:

GB 1996-3095 A 19960214
WO 1997-GB344 W 19970210
US 1997-796483 A3 19970213
US 1998-152070 A1 19980911

OTHER SOURCE(S): MARPAT 127:248122
GI



AB The invention concerns quinazoline derivs. I [X1 = bond, CO, C(R2)2, CH(OR2), S, C.tplbond.C, O, S, etc.; Q1 = Ph, naphthyl, or 5- or 6-membered heteroaryl optionally bearing 1-3 substituents; m = 1 or 2; R1 = H, halo, CF3, OH, NH2, cyano, etc.; R2 = H, alkyl; Q2 = Ph or 9- or 10-membered bicyclic heterocycle optionally bearing 1-3 substituents] and their pharmaceutically acceptable salts. Also disclosed are processes for preparation of I and salts, pharmaceutical compns. containing them, and the use of

their receptor tyrosine kinase inhibitory properties in the treatment of proliferative diseases such as cancer. Examples include syntheses of 40 compds. and various intermediates. For instance, Pd(PPh3)4-catalyzed coupling of 6-bromo-4-(3-chloro-4-fluoroanilino)quinazoline-HCl with di-iso-Pr [5-(2-morpholinoethyl)thien-2-yl]boronate (prepn. given) gave 27% title compound II. At 50 mg/kg/day in athymic nude mice with human vulval epidermoid carcinoma xenografts (cell line A-431), II gave 64% inhibition of tumor volume (vs. control) after 13 days.

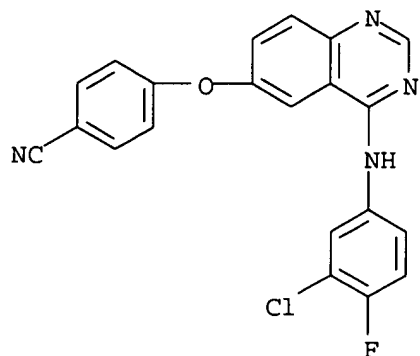
IT **195457-37-5P**, 4-(3-Chloro-4-fluoroanilino)-6-(4-cyanophenoxy)quinazoline **195457-38-6P**, 4-(3-Chloro-4-fluoroanilino)-6-(4-nitrophenoxy)quinazoline **195457-39-7P**, 6-(4-Aminophenoxy)-4-(3-chloro-4-fluoroanilino)quinazoline **195457-41-1P**, 6-[4-(Aminomethyl)phenoxy]-4-(3-chloro-4-fluoroanilino)quinazoline

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

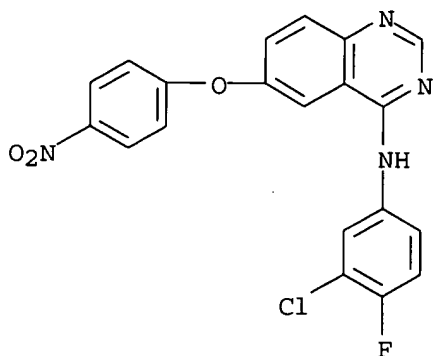
(preparation of quinazoline derivs. as antitumor agents and antiproliferatives)

RN 195457-37-5 HCAPLUS

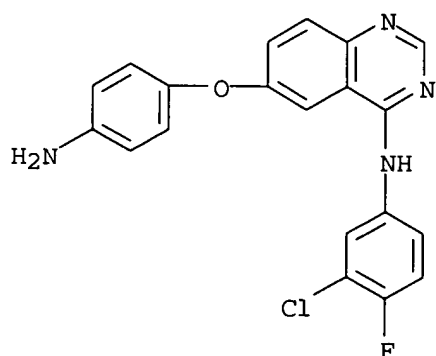
CN Benzonitrile, 4-[[4-[(3-chloro-4-fluorophenyl)amino]-6-quinazolinyl]oxy]-(9CI) (CA INDEX NAME)



RN 195457-38-6 HCAPLUS

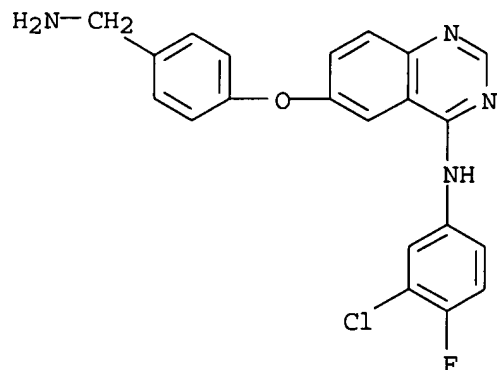
CN 4-Quinazolinamine, N-(3-chloro-4-fluorophenyl)-6-(4-nitrophenoxy)- (9CI)
(CA INDEX NAME)

RN 195457-39-7 HCAPLUS

CN 4-Quinazolinamine, 6-(4-aminophenoxy)-N-(3-chloro-4-fluorophenyl)- (9CI)
(CA INDEX NAME)

RN 195457-41-1 HCAPLUS

CN 4-Quinazolinamine, 6-[4-(aminomethyl)phenoxy]-N-(3-chloro-4-fluorophenyl)-
(9CI) (CA INDEX NAME)



IT 195457-40-0P, 4-(3-Chloro-4-fluoroanilino)-6-phenoxyquinazoline

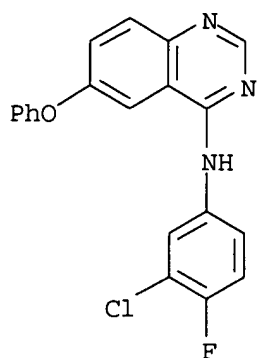
195457-42-2P, 4-(3-Chloro-4-fluoroanilino)-6-[4-(morpholinomethyl)phenoxy]quinazoline

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of quinazoline derivs. as antitumor agents and antiproliferatives)

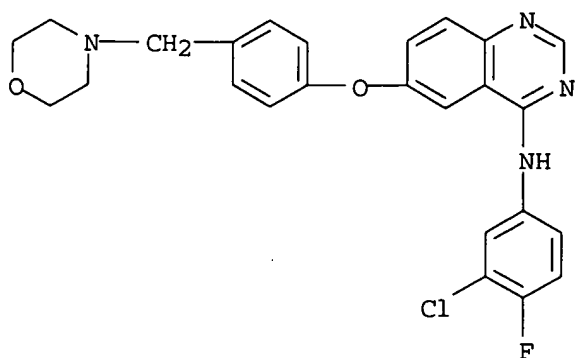
RN 195457-40-0 HCAPLUS

CN 4-Quinazolinamine, N-(3-chloro-4-fluorophenyl)-6-phenoxy- (9CI) (CA INDEX NAME)



RN 195457-42-2 HCAPLUS

CN 4-Quinazolinamine, N-(3-chloro-4-fluorophenyl)-6-[4-(4-morpholinylmethyl)phenoxy]- (9CI) (CA INDEX NAME)



L12 ANSWER 8 OF 11 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1996:467270 HCAPLUS

DOCUMENT NUMBER: 125:168006

TITLE: Preparation of 2,4-diaminoquinazolines as insecticides

INVENTOR(S): Henrie, Robert N., II; Peake, Clinton J.; Cullen, Thomas G.; Lew, Albert C.; Chaguturu, Munirathnam K.; Ray, Partha S.; Yeager, Walter H.; Silverman, Ian R.; Buser, John W.; et al.

PATENT ASSIGNEE(S): FMC Corp., USA

SOURCE: U.S., 63 pp., Cont.-in-part of U.S. Ser. No. 149,491, abandoned.

CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

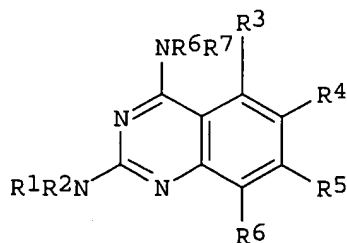
FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

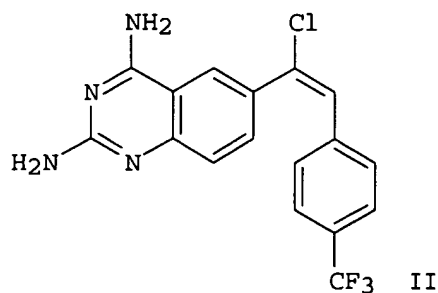
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5534518	A	19960709	US 1994-267340	19940628 <--
ZA 9401038	A	19940825	ZA 1994-1038	19940215 <--
US 5616718	A	19970401	US 1995-426541	19950420 <--
US 5874579	A	19990223	US 1996-640610	19960501 <--
PRIORITY APPLN. INFO.:			US 1993-19389	B2 19930218
			US 1993-149491	B2 19931109
			US 1994-267340	A3 19940628

OTHER SOURCE(S): MARPAT 125:168006

GI



I



II

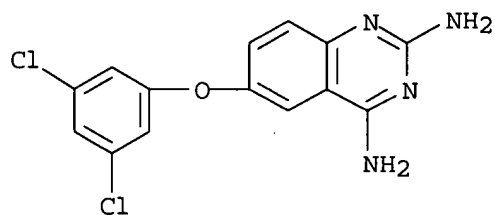
AB Title compds. [I; R1,R6 = H or alkyl; R2,R7 = H, alkyl, alkanoyl, alkoxy, carbonyl, etc.; R1R2 = O-interrupted alkylene; R1R2,R6R7 = dialkylaminomethylene, pyrrolidinomethylene, etc.; R3,R5,R6 = H halo, alkyl, alkoxy, etc.; R4 = H halo, alkyl, alkoxy, substituted aryl(oxy), NHCH2C6H4(CO2H)-4, etc.] were prepared Thus, 2-methyl-6-nitrobenzonitrile was converted in 4 steps to 2-amino-5-ethynyl-6-methylbenzonitrile which was arylated with 4-IC6H4CF3 and the product condensed with ClC(:NH)NH2.HCl to give title compound II which gave 90 and 100% kill of *Trichoplusia ni* and *Spodoptera exigua*, resp., at 30ppm foliar spray.

IT 38713-64-3P 38713-65-4P 38713-66-5P
180269-50-5P 180269-51-6P 180269-52-7P
180269-53-8P 180269-54-9P 180269-55-0P
180269-83-4P 180269-84-5P 180269-85-6P
180269-86-7P 180269-87-8P

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of 2,4-diaminoquinazolines as insecticides)

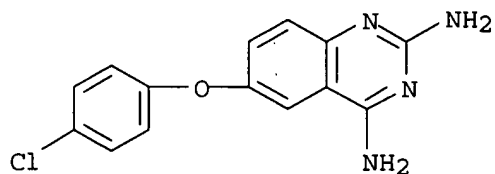
RN 38713-64-3 HCAPLUS

CN 2,4-Quinazolinediamine, 6-(3,5-dichlorophenoxy)- (9CI) (CA INDEX NAME)



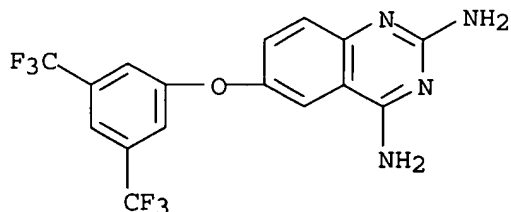
RN 38713-65-4 HCAPLUS

CN 2,4-Quinazolinediamine, 6-(4-chlorophenoxy)- (9CI) (CA INDEX NAME)



RN 38713-66-5 HCAPLUS

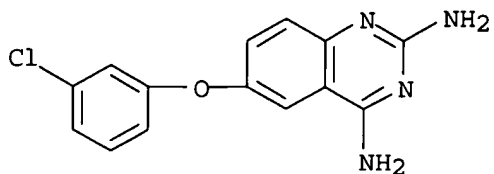
CN 2,4-Quinazolinediamine, 6-[3,5-bis(trifluoromethyl)phenoxy]- (9CI) (CA INDEX NAME)



RN 180269-50-5 HCAPLUS

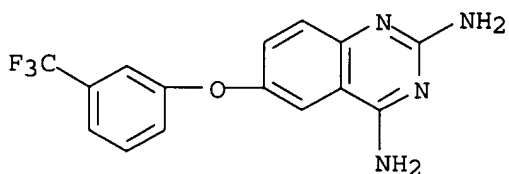
06/25/2006 10824731.trn

CN 2,4-Quinazolinediamine, 6-(3-chlorophenoxy)- (9CI) (CA INDEX NAME)



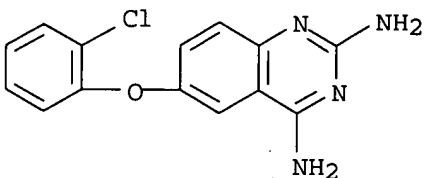
RN 180269-51-6 HCAPLUS

CN 2,4-Quinazolinediamine, 6-[3-(trifluoromethyl)phenoxy]- (9CI) (CA INDEX NAME)



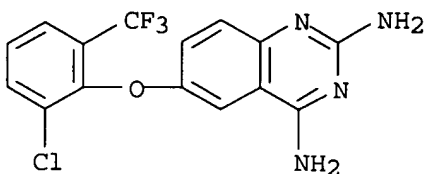
RN 180269-52-7 HCAPLUS

CN 2,4-Quinazolinediamine, 6-(2-chlorophenoxy)- (9CI) (CA INDEX NAME)



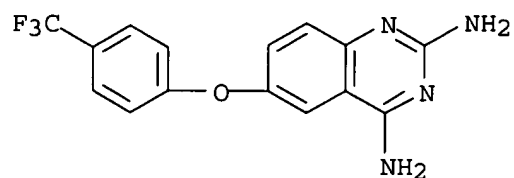
RN 180269-53-8 HCAPLUS

CN 2,4-Quinazolinediamine, 6-[2-chloro-6-(trifluoromethyl)phenoxy]- (9CI) (CA INDEX NAME)



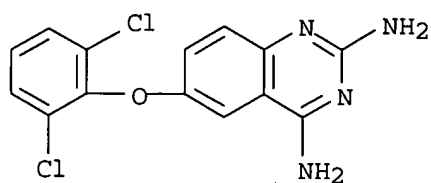
RN 180269-54-9 HCAPLUS

CN 2,4-Quinazolinediamine, 6-[4-(trifluoromethyl)phenoxy]- (9CI) (CA INDEX NAME)



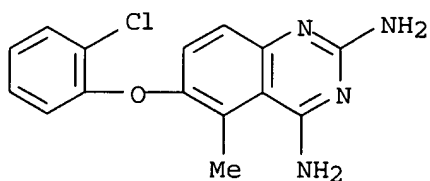
RN 180269-55-0 HCAPLUS

CN 2,4-Quinazolinediamine, 6-(2,6-dichlorophenoxy)- (9CI) (CA INDEX NAME)



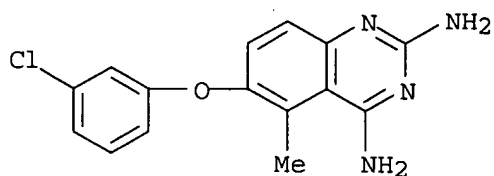
RN 180269-83-4 HCAPLUS

CN 2,4-Quinazolinediamine, 6-(2-chlorophenoxy)-5-methyl- (9CI) (CA INDEX NAME)



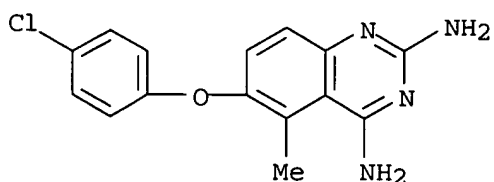
RN 180269-84-5 HCAPLUS

CN 2,4-Quinazolinediamine, 6-(3-chlorophenoxy)-5-methyl- (9CI) (CA INDEX NAME)



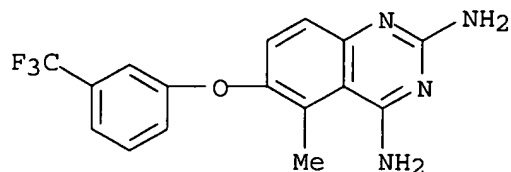
RN 180269-85-6 HCAPLUS

CN 2,4-Quinazolinediamine, 6-(4-chlorophenoxy)-5-methyl- (9CI) (CA INDEX NAME)

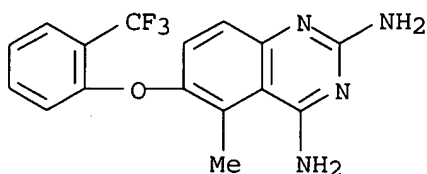


06/25/2006 10824731.trn

RN 180269-86-7 HCAPLUS
CN 2,4-Quinazolinediamine, 5-methyl-6-[3-(trifluoromethyl)phenoxy] - (9CI)
(CA INDEX NAME)



RN 180269-87-8 HCAPLUS
CN 2,4-Quinazolinediamine, 5-methyl-6-[2-(trifluoromethyl)phenoxy] - (9CI)
(CA INDEX NAME)



L12 ANSWER 9 OF 11 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1989:95260 HCAPLUS

DOCUMENT NUMBER: 110:95260

TITLE: Preparation of trans-3-[3-(3-hydroxy-2-piperidinyl)-2-oxopropyl]quinazolin-4(3H)-ones as anticoccidial agents

INVENTOR(S): Glazer, Edward A.

PATENT ASSIGNEE(S): Pfizer Inc., USA

SOURCE: U.S., 17 pp.
CODEN: USXXAM

DOCUMENT TYPE: Patent

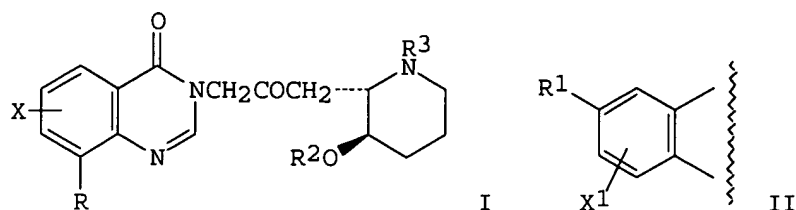
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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US 4762838	A	19880809	US 1987-67766	19870622 <--
WO 9312795	A1	19930708	WO 1985-US1685	19850830 <--
W: US				
US 4849518	A	19890718	US 1988-173207	19880324 <--
US 4920224	A	19900424	US 1989-322736	19890313 <--
PRIORITY APPLN. INFO.:			WO 1985-US1685	W 19850830
			US 1987-67766	A3 19870622
			US 1988-173207	A3 19880324

OTHER SOURCE(S): CASREACT 110:95260; MARPAT 110:95260
GI



AB The title compds. (I, II; R = Cl-4 alkylthio; R1 = CF3, Cl-4 alkylthio, cyano, 4-picolythio, 3,5-Cl2C6H3O, Y1C6H4O, Y2C6H4CH2S; R2 = R = H; X = Br, Cl, F, iodo, in 6- or 7-position; X1 = H, MeO, X, in 7- or 8-position; Y1 = H, Br, Cl, F, PhO, Y2 = Br, Cl; when X1 = H then Y1 = H) and their pharmaceutically acceptable salts were prepared as coccidiostats.

4,5,2-Cl2(O2N)C6H2CO2H was phenoxyated with 4-ClC6H4OH and the product hydrogenated to give 2-amino-4-chloro-5-(4-chlorophenoxy)benzoic acid.

The latter was cyclized by heating at 155° in H2CO to give 7-chloro-6-(4-chlorophenoxy-4(3H)-quinazolinone which was N-alkylated with allyl trans-2-(3-bromo-2-oxopropyl)-3-methoxy-1-piperidinecarboxylate to give II (R1 = 4-ClC6H4O, R2 = Me, R3 = CO2CH2CH:CH2, X1 = 7-Cl). This was stirred at room temperature in 33% HBr/HOAc to give II.2HBr (R3 = H, other groups unchanged) which was refluxed in 48% HBr to give II.2HBr (R1 = 4-ClC6H4O, R2 = R3 = H, X1 = 7-Cl). Selected I gave 90-100% control of Eimeria tenella in chicks at 25 ppm in feed.

IT 117297-62-8P 117297-63-9P 117297-64-0P

117297-65-1P 117297-66-2P 117297-67-3P

117297-68-4P 117323-95-2P 117323-96-3P

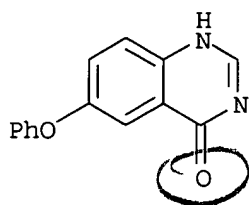
117323-97-4P 117323-98-5P 117348-69-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction of, in preparation of coccidiostats)

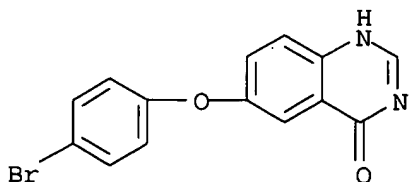
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CN 4(1H)-Quinazolinone, 6-phenoxy- (9CI) (CA INDEX NAME)



RN 117297-63-9 HCAPLUS

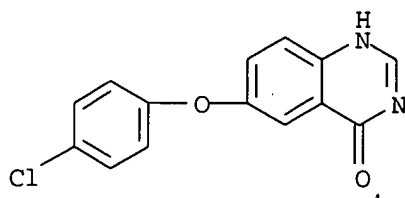
CN 4(1H)-Quinazolinone, 6-(4-bromophenoxy)- (9CI) (CA INDEX NAME)



06/25/2006 10824731.trn

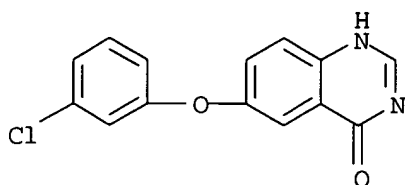
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CN 4(1H)-Quinazolinone, 6-(4-chlorophenoxy)- (9CI) (CA INDEX NAME)



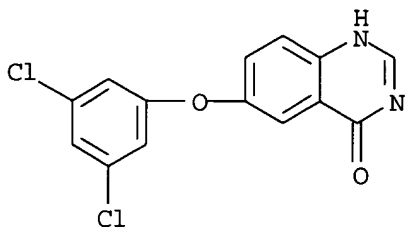
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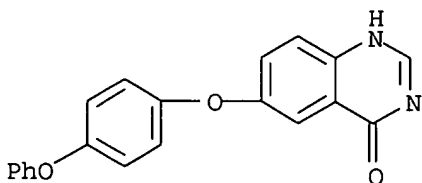
RN 117297-66-2 HCAPLUS

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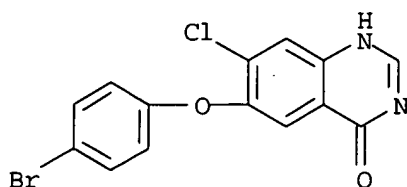
RN 117297-67-3 HCAPLUS

CN 4(1H)-Quinazolinone, 6-(4-phenoxyphenoxy)- (9CI) (CA INDEX NAME)



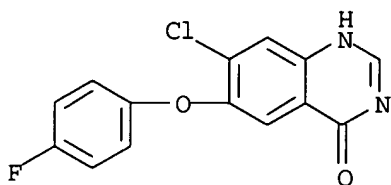
RN 117297-68-4 HCAPLUS

CN 4(1H)-Quinazolinone, 6-(4-bromophenoxy)-7-chloro- (9CI) (CA INDEX NAME)



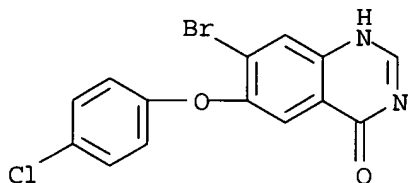
RN 117323-95-2 HCAPLUS

CN 4(1H)-Quinazolinone, 7-chloro-6-(4-fluorophenoxy)- (9CI) (CA INDEX NAME)



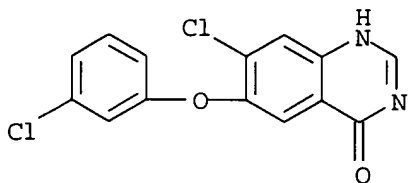
RN 117323-96-3 HCAPLUS

CN 4(1H)-Quinazolinone, 7-bromo-6-(4-chlorophenoxy)- (9CI) (CA INDEX NAME)



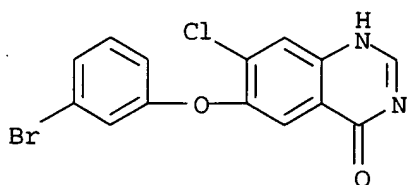
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CN 4(1H)-Quinazolinone, 7-chloro-6-(3-chlorophenoxy)- (9CI) (CA INDEX NAME)

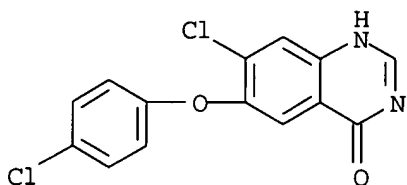


RN 117323-98-5 HCAPLUS

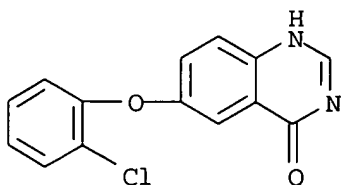
CN 4(1H)-Quinazolinone, 6-(3-bromophenoxy)-7-chloro- (9CI) (CA INDEX NAME)



RN 117348-69-3 HCAPLUS
CN 4(1H)-Quinazolinone, 7-chloro-6-(4-chlorophenoxy)- (9CI) (CA INDEX NAME)



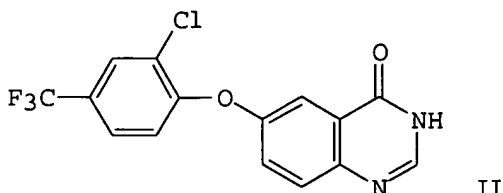
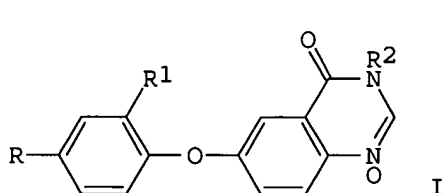
IT 117324-60-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as coccidostat intermediate)
RN 117324-60-4 HCAPLUS
CN 4(1H)-Quinazolinone, 6-(2-chlorophenoxy)- (9CI) (CA INDEX NAME)



L12 ANSWER 10 OF 11 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1983:405644 HCAPLUS
DOCUMENT NUMBER: 99:5644
TITLE: Herbicidal derivatives of 5-phenoxy-4(3H)-quinazolinone 1-oxide
INVENTOR(S): Steffens, James J.
PATENT ASSIGNEE(S): Rhone-Poulenc Agrochimie, Fr.
SOURCE: U.S., 3 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4377408	A	19830322	US 1981-286747	19810727 <--
PRIORITY APPLN. INFO.:			US 1981-286747	19810727
OTHER SOURCE(S):		CASREACT 99:5644; MARPAT 99:5644		

GI



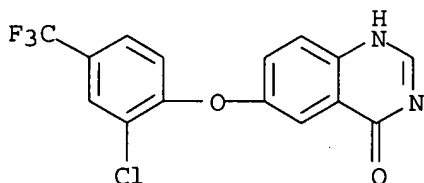
AB The herbicidal (no data) title compds. I [R = trihalomethyl; R1 = halo, R2 = H, (un)substituted C1-5 alkyl] were prepared Thus, 2,5-Cl(F3C)C6H3OC6H3(CONH2)NO2-3,4 was reduced and the resulting amine cyclized with HC(OEt)3 to give the quinazolinone II, which was oxidized with H2O, to give I (R = F3C, R1 = Cl, R2 = H).

IT **86009-58-7P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and oxidation of)

RN 86009-58-7 HCAPLUS

CN 4(1H)-Quinazolinone, 6-[2-chloro-4-(trifluoromethyl)phenoxy]- (9CI) (CA INDEX NAME)

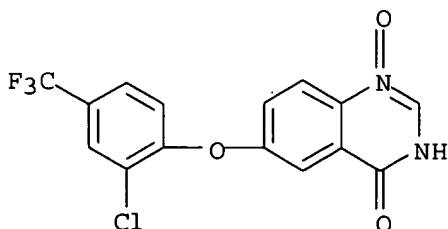


IT **86009-59-8P**

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 86009-59-8 HCAPLUS

CN 4(3H)-Quinazolinone, 6-[2-chloro-4-(trifluoromethyl)phenoxy]-, 1-oxide (9CI) (CA INDEX NAME)



L12 ANSWER 11 OF 11 HCAPLUS COPYRIGHT 2006 ACS on STN

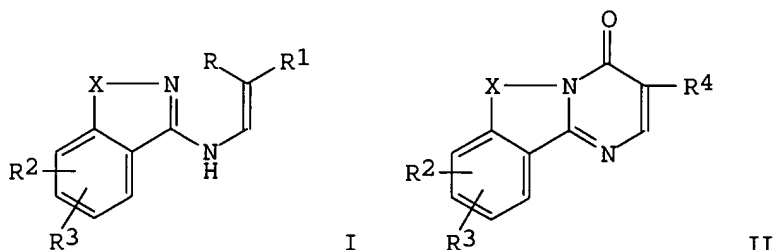
ACCESSION NUMBER: 1981:587290 HCAPLUS

DOCUMENT NUMBER: 95:187290

TITLE: Quinazoline derivatives and pharmaceutical

INVENTOR(S): compositions containing them
 Ueda, Ikuo; Kato, Masayuki; Nagano, Masanobu
 PATENT ASSIGNEE(S): Fujisawa Pharmaceutical Co., Ltd. , Japan
 SOURCE: Eur. Pat. Appl., 120 pp.
 CODEN: EPXXDW
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 30156	A1	19810610	EP 1980-304335	19801202 <--
EP 30156	B1	19840321		
R: AT, BE, CH, DE, FR, GB, IT, LU, NL, SE				
US 4377580	A	19830322	US 1980-210340	19801125 <--
AU 8064733	A1	19810611	AU 1980-64733	19801126 <--
AU 541811	B2	19850124		
DK 8005139	A	19810604	DK 1980-5139	19801202 <--
CA 1157858	A1	19831129	CA 1980-365968	19801202 <--
AT 6778	E	19840415	AT 1980-304335	19801202 <--
JP 56095174	A2	19810801	JP 1980-170459	19801203 <--
JP 05002679	B4	19930113		
ES 497426	A1	19820601	ES 1980-497426	19801203 <--
ES 507995	A1	19821001	ES 1981-507995	19811215 <--
ES 507996	A1	19821001	ES 1981-507996	19811215 <--
ES 507994	A1	19821116	ES 1981-507994	19811215 <--
US 4429126	A	19840131	US 1982-384998	19820604 <--
US 4543356	A	19850924	US 1983-455411	19830103 <--
CA 1169062	A2	19840612	CA 1983-432297	19830712 <--
JP 05294946	A2	19931109	JP 1991-201541	19910509 <--
JP 06051686	B4	19940706		
PRIORITY APPLN. INFO.:			GB 1979-41607	A 19791203
			GB 1980-31965	A 19801003
			US 1980-210340	A2 19801125
			CA 1980-365968	A3 19801202
			EP 1980-304335	A 19801202
OTHER SOURCE(S):			CASREACT 95:187290; MARPAT 95:187290	
GI				



AB The title compds. I, II [R, R1 = esterified carboxy; R2, R3 = H, alkyl, halo, NO2, NH2, alkoxy, aryloxy, etc.; R4 = H, carboxy, esterified carboxy; X = N:CR5 (R5 = H, alkyl, OH, alkoxy, alkenyloxy, dialkylamino, etc.), R6NCO (R6 = alkyl, alkenyl), etc.] were prepared Thus, stirring

4-aminoquinazoline with EtOCH:C(CO₂Et)₂ in DMF 1 h at 160° gave di-Et [(4-quinazolinylamino)methylene]propanedioate. I and II are antiallergic agents (test data given).

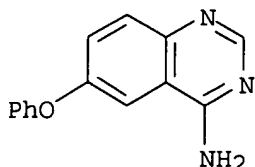
IT **79689-26-2P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction of, with alkoxymethylenepropanedioate)

RN 79689-26-2 HCAPLUS

CN 4-Quinazolinamine, 6-phenoxy- (9CI) (CA INDEX NAME)

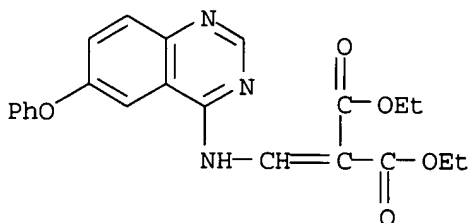


IT **79689-59-1P**

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

RN 79689-59-1 HCAPLUS

CN Propanedioic acid, [[[6-phenoxy-4-quinazolinyl)amino]methylene]-, diethyl ester (9CI) (CA INDEX NAME)



=> FIL REGISTRY

COST IN U.S. DOLLARS

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DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

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DICTIONARY FILE UPDATES: 23 JUN 2006 HIGHEST RN 889213-08-5

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*
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
*
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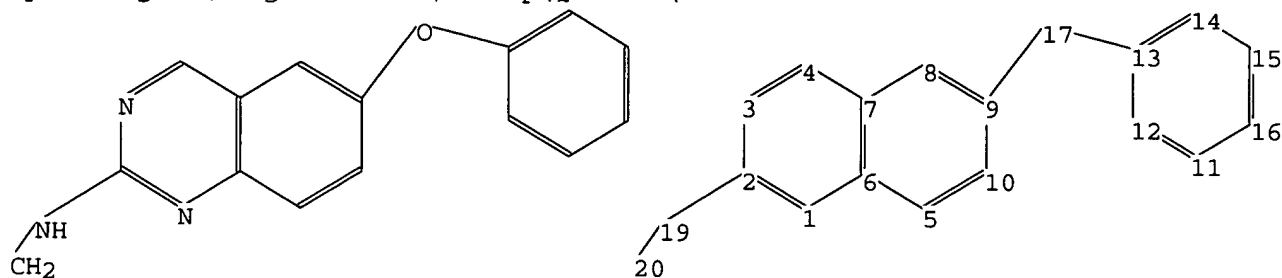
Structure search iteration limits have been increased. See HELP SLIMITS for details.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

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Uploading C:\Program Files\Stnexp\Queries\10824731b.str



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ring nodes :
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chain bonds :
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ring bonds :
1-2 1-6 2-3 3-4 4-7 5-6 5-10 6-7 7-8 8-9 9-10 11-12 11-16 12-13 13-14
14-15 15-16
exact/norm bonds :
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exact bonds :
19-20
normalized bonds :
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containing 1 : 11 :
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06/25/2006 10824731.trn

Match level :

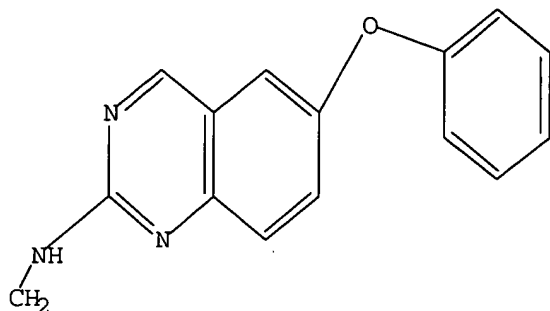
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11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:CLASS 19:CLASS 20:CLASS

L13 STRUCTURE UPLOADED

=> d l13

L13 HAS NO ANSWERS

L13 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l13

SAMPLE SEARCH INITIATED 12:11:11 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 12 TO ITERATE

100.0% PROCESSED 12 ITERATIONS

1 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 33 TO 447

PROJECTED ANSWERS: 1 TO 80

L14 1 SEA SSS SAM L13

=> s l13 sss full

FULL SEARCH INITIATED 12:11:20 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 160 TO ITERATE

100.0% PROCESSED 160 ITERATIONS

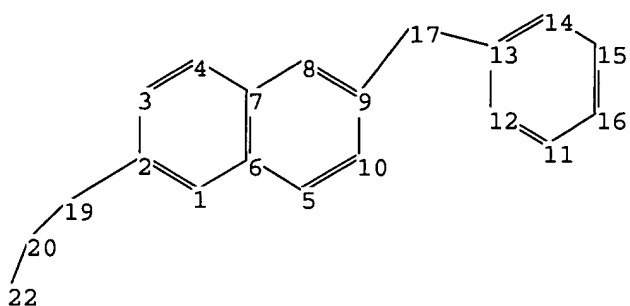
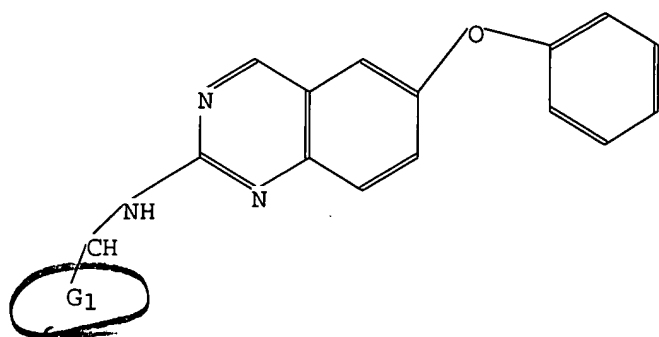
3 ANSWERS

SEARCH TIME: 00.00.01

L15 3 SEA SSS FUL L13

=>

Uploading C:\Program Files\Stnexp\Queries\10824731c.str



chain nodes :

17 19 20 22

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16

chain bonds :

2-19 9-17 13-17 19-20 20-22

ring bonds :

1-2 1-6 2-3 3-4 4-7 5-6 5-10 6-7 7-8 8-9 9-10 11-12 11-16 12-13 13-14
14-15 15-16

exact/norm bonds :

2-19 9-17 13-17 19-20 20-22

normalized bonds :

1-2 1-6 2-3 3-4 4-7 5-6 5-10 6-7 7-8 8-9 9-10 11-12 11-16 12-13 13-14
14-15 15-16

isolated ring systems :

containing 1 : 11 :

G1:Cb,Hy

Match level :

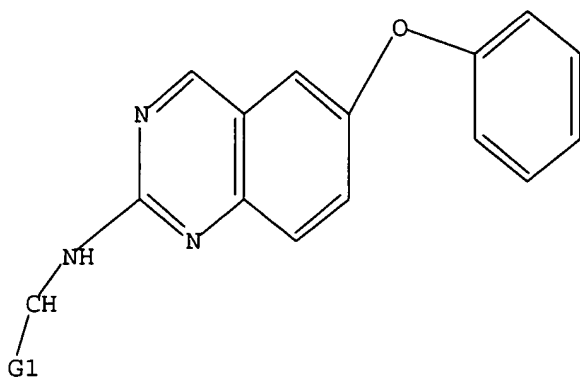
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:CLASS 19:CLASS 20:CLASS
22:CLASS

L16 STRUCTURE UPLOADED

=> d l16

L16 HAS NO ANSWERS

L16 STR



G1 Cb,Hy

Structure attributes must be viewed using STN Express query preparation.

=> s l16

SAMPLE SEARCH INITIATED 12:13:40 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 12 TO ITERATE

100.0% PROCESSED 12 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 33 TO 447
PROJECTED ANSWERS: 0 TO 0

L17 0 SEA SSS SAM L16

=> s l16 sss full

FULL SEARCH INITIATED 12:13:46 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 160 TO ITERATE

100.0% PROCESSED 160 ITERATIONS 1 ANSWERS
SEARCH TIME: 00.00.01

L18 1 SEA SSS FUL L16

=> d his

(FILE 'HOME' ENTERED AT 11:58:23 ON 25 JUN 2006)

FILE 'REGISTRY' ENTERED AT 11:58:36 ON 25 JUN 2006

L1 STRUCTURE UPLOADED
L2 1 S L1
L3 3 S L1 SSS FULL
L4 STRUCTURE UPLOADED
L5 11 S L4
L6 170 S L4 SSS FULL

FILE 'HCAPLUS' ENTERED AT 12:00:18 ON 25 JUN 2006

L7 2 S L3
L8 35 S L6

06/25/2006 10824731.trn

L9 28 S L8 AND PY<=2003
L10 0 S L9 AND P38 KINASE
L11 1 S L9 AND KINASE INHIBITORS
L12 11 S L9 AND US/PC

FILE 'REGISTRY' ENTERED AT 12:10:53 ON 25 JUN 2006

L13 STRUCTURE UPLOADED
L14 1 S L13
L15 3 S L13 SSS FULL
~~L16 STRUCTURE UPLOADED~~
L17 0 S L16
L18 1 S L16 SSS FULL

=> FIL HCAPLUS

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FULL ESTIMATED COST	335.20	786.81
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-10.50

FILE 'HCAPLUS' ENTERED AT 12:14:09 ON 25 JUN 2006

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FILE COVERS 1907 - 25 Jun 2006 VOL 145 ISS 1

FILE LAST UPDATED: 23 Jun 2006 (20060623/ED)

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=> s l15

L19 2 L15

=> s l18

L20 1 L18

=> d l19 ibib abs hitstr tot

L19 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:878161 HCAPLUS

DOCUMENT NUMBER: 141:366245

TITLE: Preparation of substituted quinazolines as p38 kinase inhibitors

06/25/2006

10824731.trn

INVENTOR(S):

Dunn, James Patrick; Goldstein, David Michael; Stahl,
~~Christoph Martin~~; Trejo-Martin, Teresa Alejandra

PATENT ASSIGNEE(S):

E. Hoffmann-La Roche AG, USA

SOURCE:

U.S. Pat. Appl. Publ., 20 pp.

CODEN: USXXCO

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

1

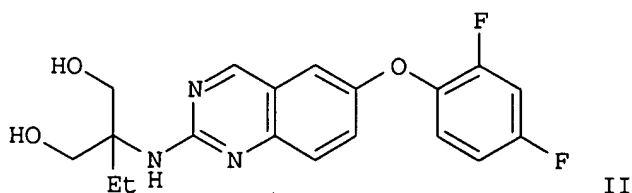
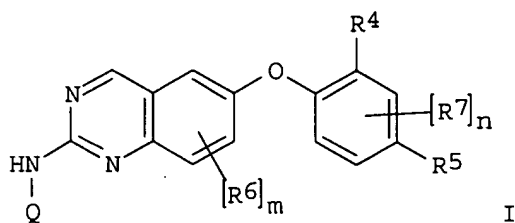
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2004209904	A1	20041021	US 2004-824731	20040415
AU 2004230209	A1	20041028	AU 2004-230209	20040408
CA 2522522	AA	20041028	CA 2004-2522522	20040408
WO 2004092144	A2	20041028	WO 2004-EP3779	20040408
WO 2004092144	A3	20050324		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1620408	A2	20060201	EP 2004-726448	20040408
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK				
BR 2004009580	A	20060418	BR 2004-9580	20040408
CN 1774425	A	20060517	CN 2004-80010341	20040408
PRIORITY APPLN. INFO.:			US 2003-463467P	P 20030416
			WO 2004-EP3779	W 20040408

OTHER SOURCE(S):

MARPAT 141:366245

GI



AB The title compds. I [R4, R5 = H, halo, CN, haloalkyl, or haloalkoxy (but are not both hydrogen); R6, R7 = alkyl, halo, CN, etc.; Q = a non-aromatic moiety; m = 0-3; n = 0-2] which are useful as p38 kinase inhibitors, were prepared and formulated. E.g., a multi-step synthesis of II, starting from Me 5-chloro-2-nitrobenzoate and 2,4-difluorophenol, which showed IC50 of <0.10 μ M against p38 MAP kinase, was given.

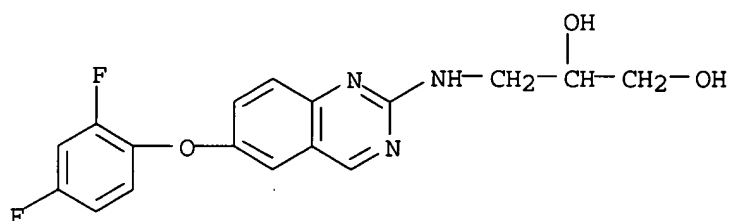
IT 778639-20-6P 778639-21-7P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of substituted quinazolines as p38 kinase inhibitors)

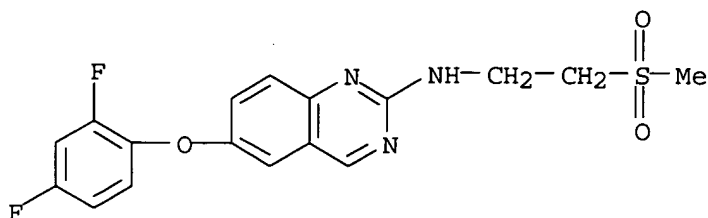
RN 778639-20-6 HCAPLUS

CN 1,2-Propanediol, 3-[[6-(2,4-difluorophenoxy)-2-quinazolinyl]amino]- (9CI)
(CA INDEX NAME)



RN 778639-21-7 HCAPLUS

CN 2-Quinazolinamine, 6-(2,4-difluorophenoxy)-N-[2-(methylsulfonyl)ethyl]- (9CI) (CA INDEX NAME)



L19 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:582372 HCAPLUS

DOCUMENT NUMBER: 142:155900

TITLE: Synthesis and phenotypic screening of a guanine-mimetic library

AUTHOR(S): Miller, Stephen C.; Mitchison, Timothy J.

CORPORATE SOURCE: Department of Cell Biology and Institute of Chemistry and Cell Biology, Harvard Medical School, Boston, MA, 02115, USA

SOURCE: ChemBioChem (2004), 5(7), 1010-1012

CODEN: CBCHFX; ISSN: 1439-4227

PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 142:155900

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

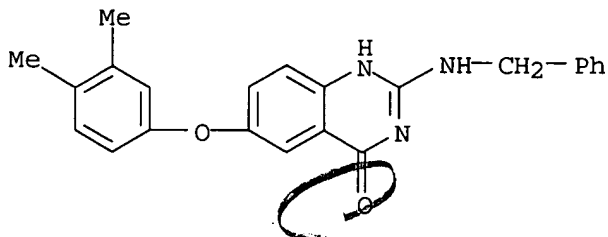
AB Guanine-derived small mols. play important roles in many aspects of cellular function. Proteins that bind guanine and its derivs. control a wide variety of cellular processes, and compds. that disrupt this binding would be valuable research tools as well as potential pharmaceuticals. A split-pool library of 270 6-substituted-2-amino-4(3H)-quinazolinones (I) (R1 = residue of thiol, phenol, or primary alcs.; R2 = aryl or alkyl; e.g. R1 = 3,4-dimethylphenyl, R2 = 3,4,5-trimethoxyphenyl, benzyl; R1 = isobutylthio, R2 = 3-acetylphenyl; R1 = cyclohexylthio, R2 = 4-chlorophenyl) was prepared by aza-Wittig-mediated solid-phase synthesis which involves (1) nucleophilic aromatic substitution of a resin-bound 5-fluoro-2-nitrobenzamide with a variety of thiols, phenols, and primary alcs., (2) generation of a resin-bound iminophosphorane (II) (P = resin) by treatment with Ph3P/Cl3CCCl3/imidazole (3 h, 4°), (3) aza-Wittig reaction of the iminophosphoranes with one of 15 isocyanates (R2-NCO) to yield a carbodiimide (III) (P = resin) followed by intermol. O-attack instead of the desired N attack to the carbodiimide to yield an 4-imino-4H-3,1-benzoxazine (IV), and (4) DBU-mediated isomerization to the desired 2-amino-4(3H)-quinazolinone (V) (P = resin) followed by resin cleavage. The compds. I were cell-permeable guanine-mimetics and screened for (a) the effect on the cytoskeleton and cell cycle progression by incubating the compds. with BS-C-1-(monkey) cells for 6 h, followed by fixing and staining for actin, DNA, and microtubules and (b) disruption of cellular trafficking. For example, I (R1 = isobutylthio, R2 = 3-acetylphenyl) disrupted both the actin and microtubule cytoskeleton, but did not arrest cells in mitosis.

IT 828261-87-6P

RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(solid-phase synthesis and phenotypic screening of guanine-mimetic library via aza-Wittig reaction of iminophosphoranes with isocyanates and DBU-mediated isomerization iminobenzoxazines)

RN 828261-87-6 HCAPLUS

CN 4(1H)-Quinazolinone, 6-(3,4-dimethylphenoxy)-2-[(phenylmethyl)amino]-
(9CI) (CA INDEX NAME)



REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d 120 ibib abs hitstr tot

L20 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:582372 HCAPLUS
DOCUMENT NUMBER: 142:155900
TITLE: Synthesis and phenotypic screening of a
guanine-mimetic library
AUTHOR(S): Miller, Stephen C.; Mitchison, Timothy J.
CORPORATE SOURCE: Department of Cell Biology and Institute of Chemistry
and Cell Biology, Harvard Medical School, Boston, MA,
02115, USA
SOURCE: ChemBioChem (2004), 5(7), 1010-1012
CODEN: CBCHDH; ISSN: 1439-4227
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 142:155900
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Guanine-derived small mols. play important roles in many aspects of cellular function. Proteins that bind guanine and its derivs. control a wide variety of cellular processes, and compds. that disrupt this binding would be valuable research tools as well as potential pharmaceuticals. A split-pool library of 270 6-substituted-2-amino-4(3H)-quinazolinones (I) (R1 = residue of thiol, phenol, or primary alcs.; R2 = aryl or alkyl; e.g. R1 = 3,4-dimethylphenyl, R2 = 3,4,5-trimethoxyphenyl, benzyl; R1 = isobutylthio, R2 = 3-acetylphenyl; R1 = cyclohexylthio, R2 = 4-chlorophenyl) was prepared by aza-Wittig-mediated solid-phase synthesis which involves (1) nucleophilic aromatic substitution of a resin-bound 5-fluoro-2-nitrobenzamide with a variety of thiols, phenols, and primary alcs., (2) generation of a resin-bound iminophosphorane (II) (P = resin) by treatment with Ph3P/Cl3CCl3/imidazole (3 h, 4°), (3) aza-Wittig reaction of the iminophosphoranes with one of 15 isocyanates (R2-NCO) to yield a carbodiimide (III) (P = resin) followed by intermol. O-attack instead of the desired N attack to the carbodiimide to yield an 4-imino-4H-3,1-benzoxazine (IV), and (4) DBU-mediated isomerization to the desired 2-amino-4(3H)-quinazolinone (V) (P = resin) followed by resin cleavage. The compds. I were cell-permeable guanine-mimetics and screened for (a) the effect on the cytoskeleton and cell cycle progression by incubating the compds. with BS-C-1-(monkey) cells for 6 h, followed by fixing and staining for actin, DNA, and microtubules and (b) disruption of cellular trafficking. For example, I (R1 = isobutylthio, R2 = 3-acetylphenyl) disrupted both the actin and microtubule cytoskeleton, but did not arrest cells in mitosis.

IT 828261-87-6P

RL: BSU (Biological study, unclassified); SPN (Synthetic preparation);
BIOL (Biological study); PREP (Preparation)

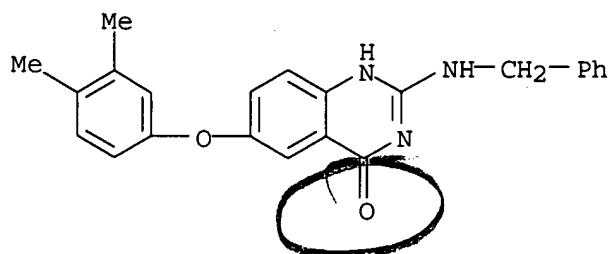
(solid-phase synthesis and phenotypic screening of guanine-mimetic library via aza-Wittig reaction of iminophosphoranes with isocyanates and DBU-mediated isomerization iminobenzoxazines)

RN 828261-87-6 HCAPLUS

CN 4(1H)-Quinazolinone, 6-(3,4-dimethylphenoxy)-2-[(phenylmethyl)amino]-
(9CI) (CA INDEX NAME)

06/25/2006

10824731.trn



REFERENCE COUNT:

9

THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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SESSION

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807.20

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

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-12.75

STN INTERNATIONAL LOGOFF AT 12:15:27 ON 25 JUN 2006